WS-PGRADE Portal User Manual

Version 3.6.5

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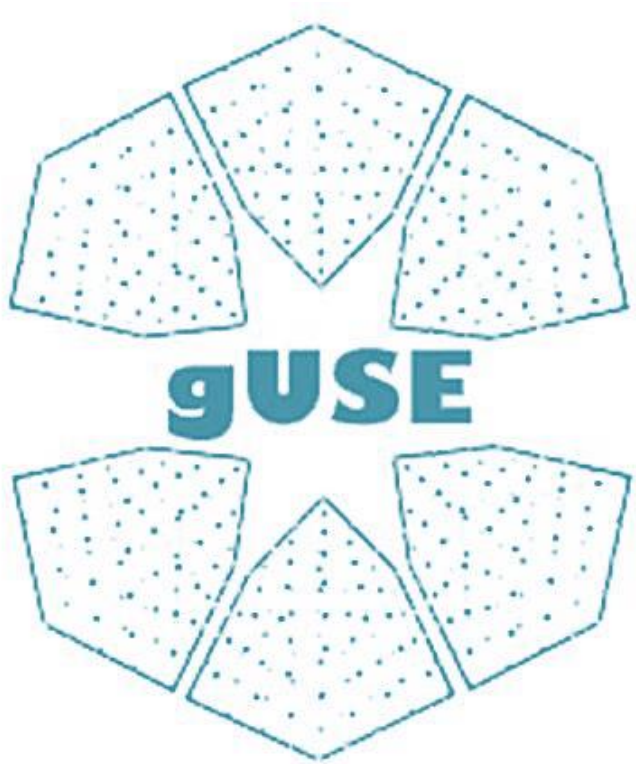
WS-PGRADE PORTAL USER MANUAL

WS-PGRADE PORTAL COOKBOOK

Docs for User Series



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Laboratory of Parallel and Distributed Systems

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About this Manual

The gUSE/WS-PGRADE User Manual is a detailed guide and description of WS-PGRADE Portal at user level. The WS-PGRADE Portal, developed by Laboratory of Parallel and Distributed Systems at MTA SZTAKI, is a web portal of the grid and cloud User Support Environment (gUSE). It supports development and submission of distributed applications executed on the computational resources of various distributed computing infrastructures (DCIs) including clusters (LSF, PBS, MOAB, SGE), service grids (ARC, gLite, Globus, UNICORE), BOINC desktop grids as well as cloud resources: Google App Engine, CloudBroker-managed clouds as well as EC2-based clouds.

How this Manual is Organized

This Manual has the following structure:

1. The **Main Part** which comes directly after the **Release Notes,** explains the basic concepts and terms to use WS-PGRADE portal. This section covers the ultimate element of WS-PGRADE usage.
2. The **Menu-Oriented Online Help** introduces the practical use of WS-PGRADE menus and functions.
3. The third section, the **Jump Start in the Development Cycle** gives you a big picture about the workflow configuration and submission process (if you search for detailed description of various job configuration and submission, download and use the *WS-PGRADE Cookbook*)

The document uses light purple color for **notifications** and light orange for **pitfalls** and **warnings**.

Release Notes

Release Notes to Version 3.6.5

The only one but important change in this version is the improvement of **EC2-based direct cloud access**. This modified solution is more comfortable to use, the administrators don’t need to install Euca2ools to prepare master DCI Bridge and the users can use more cloud services from one portal by this solution.

More details:

- in chapter 18 within Menu-Oriented Online Help
- in section 5.19 within DCI Bridge Manual
- in chapter VI within Admin Manual.

Release Notes to Version 3.6.4

The main improving in version 3.6.4 is to support the job submission by the **SHIWA Submission Service**. The web service based SHIWA Submission Service replaces the old GT4-based GEMLCA Service and enables execution of workflows based on different workflow engines. Therefore you can use in WS-

PGRADE various workflows from various communities developed in various engines. All of these workflows are stored in the central workflow repository (called SHIWA Workflow Repository). Workflows have been stored in the SHIWA Workflow Repository can be explored by several ways, for example the WS-PGRADE offers for workflow browsing a runtime built-in look up tool, the SHIWA Explorer. (You find related user-level documentation in chapter 8 within Main part, in chapter 23 within the Menu-Oriented Online Help, administrative information in chapter 2.10 of DCI Bridge Manual as well as in chapter VIII of Admin Manual.)

Other changes:

- From this release the DCI Bridge handles HTTPS-based inputs and outputs beside HTTP-based I/O. (You can read about the Additional Settings in case of Not Trusted Certification in chapter IX within Admin Manual.)
- From this version the CloudBroker entities (exactly: the wrapper applications that run executables) are identified by ID instead of names. This change affects the CloudBroker-based middleware setting in case of applying own wrapper.
- Additional minor bug fixes are in CloudBroker portlet development, in error log handling (SourceForge bug report: #218) and in Data Avenue portlet development, in download function.
- Solving the next problem: Callback functionality marks successful jobs as error jobs (SourceForge bug report: #222)
- Improved Install Wizard tool: fixes a number of class loading issues, enables using already available databases for the deployment.

Finally, an important improvement is the Single Job Wizard, a new development based on gUSE/ASM API for simplifies workflow creation and execution in the simplest case, if the workflow contains one job only. This web application is not a part of gUSE 3.6.4 package but a separate solution of ASM. (All related information about Single Job Wizard can be found at ASM menu of gUSE SourceForge site: https://sourceforge.net/p/guse/asmsp/wiki/Single%20Job%20Wizard/ and a short description in chapter X. within Admin Manual)

Release Notes to Version 3.6.3

The release 3.6.3 of gUSE contains three main changes:

First of all, there are more improvements in the file commander called **Data Avenue** first released in version 3.6.0:

- Capability of automated **user ticket generation** to use Data Avenue within portals
- Admin ticket request form (see details about admin ticket request in *chapter VII* within *the Admin Manual*)
- Support for S3 protocol
- Changes in **Favorite** settings as well as minor changes in design
- Improved file upload
- Changes in **backend** (in Data Avenue blacktop service):

- Security improvements: in-memory credentials, alias credentials are now encoded and deleted on expiration
- Use of JSAGA version 1.0.0
- Interface naming made conform to OGSA-DMI
- Improved logging
- Bug fixes

More about Data Avenue you find in *chapter 21 within Menu-Oriented Online Help* as well as in *chapter VII of Admin Manual*.

The two other developments come from the gUSE community (from Ruđer Bošković Institute, Zagreb and from Eberhard Karls University, Tübingen): the supported cluster set enriched by the development of submitters to SGE (Sun Grid Engine) and MOAB clusters. The configuration and operation of both submitters is very similar to PBS and LSF. (Details: *Portal User Manual - chapter 6.2.20 and chapter Public Key; DCI Bridge Manual – chapter 2.7 and 2.19.)*

There is a change in logging mechanism of gUSE as well: from this version the logging is possible with Apache log4j. By the application of log4j is the debugging and troubleshooting of gUSE components will be easier by the developers and administrators. (See details in chapter *Logging with log4j* within the *Additional Enhancement* of *Admin manual*.)

Additionally, this release is also includes a bug fixing: the solving of UNICORE jobs problem - these jobs didn't work with XtreemFS remote ports earlier (SourceForge bug report: #211).

Release Notes to Version 3.6.2

There are more changes in release 3.6.2:

- The main improvement in this version is the **solution of direct cloud access**. By this development the user can easily submit jobs directly to the cloud without any brokering support. To this the user just need to own and use valid authentication data received from cloud provider. (See details in *Chapter 18* within the *Menu-Oriented Online Help* as well as in *chapter 6*.) However, there is needed some preliminary administration tasks for proper using of direct cloud access. (About these tasks and additional considerations you find details in *chapter VI* of *Admin Manual* and in *chapter 2.18* of *DCI Bridge Manual*.)
- Another relevant change is the **solution of remote definition and using of executables**. This new feature of WS-PGRADE job configuration enables users to add remote URL of the executable. (The local uploading of executables was only supported earlier.) Additionally, the supported protocol set to define remote sources of inputs is extended as well. (See details in chapter 14.)
- An additional minor change: the unnecessary temporary files will be automatically deleted from directories of WS-PGRADE and WFI components after saving workflow configuration as well as after workflow submission.

Further bug fixes:

- Solving the job saving problem in case of CloudBroker (SourceForge bug report: #121).
- Adding missing messages in case of CloudBroker (SourceForge bug report: #123).
- Solving the lost arguments problem in case of CloudBroker job configuration (SourceForge bug report: #134).
- Bug fixing by the UNICORE gUSE community: it solves the problem of UNICORE submitter that generates incorrect number of cores (SourceForge bug report: #192).

Release Notes to Version 3.6.1

The main improvement in gUSE v3.6.1 is the solution for debugging of job submissions by applying breakpoints in WS-PGRADE workflows. By this tool the users can interact with workflows at runtime: they can directly influence and change workflow's submission processes and results by enabling or prohibiting the progress of job instances at breakpoints (for more details see chapter 13).

From this version the Graph Editor can be used with the latest Java upgrade (Java 1.7.0_45) as well.

Additionally, a minor change is a bug fixing (related bug report on SourceForge: #184): The (jobtype=single) will be set in GT5 RSL, when the property "Kind of binary:" is configured to "Sequential".

Release Notes to Version 3.6.0

The main change in this version is a developed tool called Data Avenue that integrated the function of Data Avenue web service as a new portlet into WS-PGRADE portal. Data Avenue is a useful file commander for data transfer, enabling easy data moving between various storages services (such as grid, cloud, cluster, supercomputers) by various protocols (HTTP, HTTPS, SFTP, GSFTP, SRM). The using of Data Avenue is similar to other well-known file commanders (e.g. Total Commander or Midnight Commander): you can use a simple two-panel (source and destination) form to copy, delete, download, upload etc. (for more details see chapter 20 within *Menu-Oriented Online Help*).

And one more new development: the overall billing and pricing information menu (*CloudBroker Billing*) in WS-PGRADE to support the CloudBroker-specific (pay-per-use) job submission (for more details see chapter 17.2 within *Menu-Oriented Online Help*).

Minor changes, bug fixes and other error solving to feature requests:

- Integrated DCI Bridge: a common bridge instance may support gLite and UNICORE.
- *voms-proxy-certificate* expiration time ("Proxy Valid") option can be set for each gLite VO in the DCI Bridge.
- Workflow name length limitation to 250 characters is checked (SourceForge bug report: #169).
- Admin can set default JDL parameters for the VOs.
- Extension the effect of the Delete all instance command to the workflow instances being in "suspended" status.
- Fixing the problem of the workflow submission related automatic email notification.
- Fixing the problem that the DCI_BRIDGE did not forward the abort requests of the user toward the DCIs in some cases.

- Solving the problem that a job might show false “running” state in case of the missing public key on the remote PBS resource (SourceForge bug report: #167)
- Correcting the values of the “Debug mode” in the “Settings” pane of the DCI Bridge (SourceForge bug report: #170).
- Correcting the problem that the creation of a workflow may fail without proper error message (SourceForge bug report: #161).
- Correcting the problem of the missing error message in the case of a missing PBS connection (#132).
- Correcting a problem experienced when the free input port of a job was connected to the result of a database query (SourceForge bug report: #77).
- Correcting the file size limit extension problem: WS-PGRADE warns if the size of the file to be uploaded is larger than the configured maximum (SourceForge bug report: #71).
- Correcting the problem that LFC portlet might use invalid certificates after registering of an internal server (SourceForge bug report: #15).
- New JDL tags supporting a different kind of MPI submission: If the user wants to avoid the obligatory running of the standard “mpirun” then she defines her job as “normal” instead “MPI” and in the JDL extension of the job definition describes the needed parameter by the new tags “SMPGranularity” and “CPUnumber” (SourceForge bug reports: #47, #53, #55, #56).

Release Notes to Version 3.5.8

The major improvement in version 3.5.8 is the internal system performance optimization for job execution. This internal reorganization of exchanging information between WS-PGRADE and the various gUSE components significantly increases the performance of WS-PGRADE portal. The changes mainly concern the background processes, only two minor visual changes appears on portal user interface: in *Workflow/Concrete/Details* function and in *Storage* function (the updated description of this two parts of the portal you can see in chapter *3.1* and *5* within section *Menu-Oriented Online Help*).

Other changes:

- The administrative configuration of Remote API is easier than earlier: you can set it in the WS-PGRADE portal. (See the details about the Remote API configuration and usage in *RemoteAPI_Install_Manual.pdf* and in *RemoteAPI_Usage.pdf.* You can also find some examples for using Remote API in the *RemoteAPI_Usage_Examples.zip* in the *Documentation* folder.)
- The maximum quota size belonging to a portal user for workflow is increased to 10000 MB (the earlier limit was 5000 MB). About the quota setting see chapter *The Internal Services* in the *Administrator Manual*.
- In the new version (v3.4.5) of ASM new features were implemented (getting/setting resource of a job; getting/setting number of input files uploaded as paramInputs.zip; setting remote output path for a given output port; getting content of an input file). The ASM v3.4.5 is compatible with gUSE from version 3.5.8, and not compatible with older versions. (For upgrading from v3.4.4 to v3.4.5 see the *Portal_Upgrade_Manual_v3.5.8.pdf*. You can find more details about ASM usage in the *ASM_Developer_Guide_v3.4.5.pdf.*)

Additionally, this release comes with more error fixings. The whole list:

- Error fixing of *Suspend all* button functionality (bug number on gUSE SourceForge: #139)
- Error fixing of *Suspend* button (bug #138)
- Solving of WFI monitor error (bug #130)
- Installation error fixing in version 3.5.3 (bug #107)
- Problem solving of *paramInputs.zip* file (bug #95)
- Problem solving in output transfer between two jobs (bug #84)
- Error fixing of *Delete Old Instances* option (bug #82)
- Problem solving the low level of user quota (bug #81)
- Solving the vulnerability problem in cross scripting (bug #78)
- Bug fixing of live file generation from database (bug #77)
- Error fixing of BOINC jobs error status information (bug #144)
- Problem solving in configuring “binaries” for REST middleware (bug #142)
- Bug fixing of filtering during add operation of GT2 resource (bug #141)
- Problem solving of disturbing line separators in public key (bug #131)
- Solving the gLite-based remote file opening problem (bug #128)
- Fixing the visibility of the *Security/CloudBroker* menu for power- and end users. (bug #148)
- Error fixing in resubmission of aborted LSF jobs (bug #159)
- Solving the too short proxy lifetime problem (bug #125)
- ASM-specific bug fixings (bug #164 and #165)

Release Notes to Version 3.5.7.1

In gUSE/WS-PGRADE version 3.5.7.1 all the patches of 3.5.7 are applied, and additionally, the following bugs are fixed:

- Uploading via LFC portlet (list of available storage elements is empty) (bug #143)
- Providing proper version in a SHIWA Bundle to be exported (mentioned in bug #149)
- Filtering of importable SHIWA bundles (bug #147)

Release Notes to Version 3.5.7

The main change in gUSE/WS-PGRADE version 3.5.7 is the fast statistical data processing and providing mechanism in Statistics function that loads the gUSE database at lower level than earlier and exploits the resources more effectively than in the previous gUSE versions (see chapter 11 to read more about *Collection and Visualization of Usage Statistics*).

Additionally, the following bugs are fixed:

- GEMLCA-based default input file error fixing (bug number on gUSE SourceForge: #135)
- Bug fixing in output files downloading from Storage/Local (bug #89)
- Solving of disappearing problem of workflows, graphs, and storage after restart (bug #87)
- Solving of minor issue after a refresh of graph list (bug #69)

Release Notes to Version 3.5.6

The main improvement in version 3.5.6 is the development in WS-PGRADE workflow export/import to/from Remote SHIWA Repository. From this version you can share your workflow to SHIWA project community in WS-PGRADE format and in SHIWA IWIR format as well (the latter solution is useful if you want to use your workflow by other workflow management systems than WS-PGRADE. However, for successful sharing, before in IWIR format export – unlike in WS-PGRADE format - your workflow can fit some rigorous preliminary conditions. For details see chapter 11 in Menu-Oriented Online Help.). Therefore the shared workflows can be imported from remote repository to WS-PGRADE portal environment in well-known WS-PGRADE implementation format or in IWIR format. (For details see chapter 7 and 11 in Menu-Oriented Online Help.)

Error fixes:

- Job submission error fixing. (SourceForge bug number #120)
- A job status query bug fixing. (bug #118)
- gLite MPI-type job submission error fixing. (bug#105)
- Error fixing in WS-PGRADE Upload certificate feature: it didn't work if in the certificate (p12) file name was a space. The error fixed. (bug #104)
- Confusing error fixing when using PBS without configuration of SSH keys. (bug #100)
- Fixing the DCI Bridge BOINC plugin error. (bug #93)
- Solving the Liferay 6.1.1 and the Concrete workflow saving problem. (bug #80)

Release Notes to Version 3.5.5

From this version users with corresponding rights can create robot permission association for every supported resource type in gUSE/WS-PGRADE to identify trusted applications. Therefore, any users can easily submit workflows identified by robot permission without dealing with any authentication data. (For details see chapter 19 in *Menu-Oriented Online Help* as well as the *Administrator Manual* where you find a description about the robot permission related logging of job submissions in the section *Additional Enhancements.*)

Release Notes to Version 3.5.4

The main improvements in version 3.5.4:

New features:

- A priori cost estimation and a posteriori real cost reporting feature for payable cloud related job submissions is included. (For details see chapter 17 in *Menu-Oriented Online Help*)
- Portal installations can subscribe to a common Google map based server advertising the included installations (*https://guse.sztaki.hu/MapService*).

Error fixes:

- Instances of workflows are not dragged with during workflow export (and consequently during workflow import).
- Thorough check of workflow related user defined names (patches in version 3.5.2 and in version 3.5.3) is part this version.
- The workflow configuration can be performed on the IE9 browser as well.
- Portal cache stored CloudBroker-related static information is refreshed at a 30 minute rate frequency.

Release Notes to Version 3.5.3

The main improvements in this version:

- There are some developments in system performance optimalization at DCI Bridge side. The main result is for users the significantly faster job processing and submission.
- gUSE/WS-PGRADE supports the EMI-UI v1 and v2, as well. Therefore, for using gLite middleware to run your workflows you can use the very simple Security/Upload function in WS-PGRADE to upload authentication data to MyProxy server (for details see chapter 2.1 in *DCI_Bridge_Manual_v3.5.3.pdf*).
- There are also new developments and bug fixing in WS-PGRADE for CloudBroker-specific job creation and submission.
- You can use new middlewares (REST and HTTP) for job configuration when you configure your job as Service in WS-PGRADE (for details see chapter 18 in *Menu-Oriented Online Help*, as well as the *DCI_Bridge_Manual_v3.5.3.pdf*).
- You can start/stop the gUSE by some useful scripts instead of longer manual step sequence. (For more information see the first section of *gUSE_Admin_Manual.pdf*)

Other changes:

- Configurational interface improvement in DCI Bridge in case of Globus (GT2,4,5) and gLite middlewares. (See the details in *DCI_Bridge_Manual_v3.5.3.pdf*)
- Shorter CloudBroker-based parametric generator and collector job running time.
- Bug fixing in DCI Bridge - in GT2/4/5 configuration, gLite status handling on EMI-UI v2, GT5 RSL modification and error handling, PBS/LSF job resubmission correction, PBS/LSF collection status query (fixing the bugs #57, #58, #65, #79).

Release Notes to Version 3.5.2

From this version gUSE/WS-PGRADE supports the workflow export/import to/from SHIWA project Workflow Repository where you can share workflows of different workflow systems. The details and the exact conditions of sharing workflows you can read in the section *Menu-Oriented Online Help*, in chapter 7 and chapter 11. (You can find the concerned functions in WS-PGRADE under menus Workflow/Import and Workflow/Concrete/Export.)

Release Notes to Version 3.5.1

In this version the job configuration capabilities of CloudBroker menu in WS-PGRADE are extended: Beside the existing opportunity of software selection from available software list of CloudBroker Repository, users can upload and use their own executable code for job submission through CloudBroker. Therefore, users can define access to their own cloud resources via CloudBroker as well as they can define applications over custom-prepared virtual machine images. You can read about the CloudBroker menu in chapter 17 within the section *Menu-Oriented Online Help.* (You can find the related functions in WS-PGRADE under Security/CloudBroker menu and during the Workflow creation process.)

Further changes:

- There is statistics in DCI Bridge user interface about job related queues.
- Further improvement of DCI Bridge user interface: new features are in resource settings (in job status handling is the “Callback URL for status sending” option and in error debugging is the opportunity to enable “Debug mode”) More about this development you can read in DCI Bridge Administrator Manual in chapter 1.2.
- A bug constraining for uploaded job input files in 10 MB has been removed.
- WFI bug fixed

Release Notes to Version 3.5.0

From this version

- the UNICORE middleware support is updated, and supports IDB tools. (About UNICORE you find information in chapter 6.2.13 and in DCI Bridge Administrator Manual, in chapter 2.5)
- opportunity to submit jobs to CloudBroker is available. (see chapter 17 in section *Menu-Oriented Online Help*). You can find the related functions in WS-PGRADE under Security/CloudBroker menu and during the Workflow creation process.

Other modifications:

- ARC bugfix
- Statistics bugfix
- DCI-Bridge handles the resources even in case of "https://host.com/service" format correctly. (GEMLCA - GT4 problem fixed)

Release Notes to Version 3.4.8

From this version the GT5 (Globus Toolkit 5) as DCI/grid type is supported as well. You can read about this in chapter 6 as well as in chapter 2.4 in DCI Bridge Administrator Manual. (You meet GT5 resource setting in a particular case in WS-PGRADE portal at the Workflow configuration process, in Workflow/Concrete/Configure function.)

Release Notes to Version 3.4.7

The gUSE/WS-PGRADE 3.4.7 introduces a visual feedback for users about relative long time running processes. Additionally, the visual forms of most messages and other dialog elements are modified and streamlined.

Release Notes to Version 3.4.6

The changes in version 3.4.6:

- Service wizard: a new gUSE tool for service checking and configuration at deployment process of gUSE.
- From this gUSE version the v6.1 is the only one supported Liferay Portal version for WS-PGRADE/gUSE installation.

Release Notes to Version 3.4.5

From this version SHIWA Repository can be connected to WS-PGRADE/gUSE.

Release Notes to Version 3.4.4

The improvement is the solution of EDGI VO support: support for gLite VOs that are extended with DG-based EDGI technology. Therefore gUSE/WS-PGRADE users can run applications on EDGI infrastructure.

Additional changes:

- End user interface bug fixed
- Certificate interface bug fixed (deleting CERT and assigning CERT to another grid)
- DCI Bridge modification: In case of BOINC and GBAC job submission: instead of assigning core URL to DCI Bridge, DCI Bridge gets job I/O files with “Public URL of Component” setting (in case of remote file access)
- Saving of workflow type and service type job configuration bug fixed.

Last but not least a new tool (gUSE Install Wizard) created that eases the installation of WS-PGRADE/gUSE. This tool offers the following installation scenarios:

- local: all gUSE and WS-PGRADE (along with Liferay) services are deployed on one machine,
- distributed: frontend (WS-PGRADE, Liferay) and backend (DCI Bridge, WFI, WFS, ...) service sets are deployed on two different machines.

Release Notes to Version 3.4.3

The main change in gUSE 3.4.3 is the support of the new version (v6.1) of Liferay Portal that is the portal technology of WS-PGRADE.

Other changes:

- User File Upload bug fixed.
- Collector handling bug fixed.

- Quota handling fixed.

Release Notes to Version 3.4.2

The changes in version 3.4.2:

- gLite, ARC and UNICORE can also run on EMI User Interface machines. NOTE: gLite installed on an EMI UI needs proxy with X509v3 extensions but it is not supported by the Certificate menu's "Upload authentication data to MyProxy server" function. You can upload your proxy to a myproxy server for example with the following command:

  ```
  myproxy-init -s myproxy.server.hostname -l MyProxyAccount -c 0 -t 100
  ```

- ARC job handling bug fixed.
- LSF bug fixed.
- Storage connection handling fixed.

Additionally, the user manual description is extended by the exact steps of user management process.

Release Notes to Version 3.4.1

The changes in version 3.4.1: Collection and visualization of usage statistics. These additions enable users and administrators to retrieve statistics on the portal, user, DCI's, resources, concrete workflows, workflow instances, and individual jobs from the workflow graph.

Release Notes to Version 3.4

There are some important changes in version 3.4:

- The backend of the gUSE has been replaced by a new uniform service, the DCI Bridge. It replaces the former "Submitters" and serves as a single unified job submission interface toward the (mostly remote) resources (DCI-s) where the job instances having been created in the gUSE will be executed. Together with the introduction of the DCI Bridge the inserting of resources supported by uprising new technologies (clouds and other services) will be simpler and better manageable.
- The following resource kinds (middlewares) appeared among the supported new technologies – via the DCI Bridge: UNICORE, GBAC, GAE (See the listing of all supported resources here.)
- The new Assertion menu supports the creation and upload of the certificate like assertion file. The assertion technology is the base authentication and authorization method of the UNICORE middleware used in the D-GRID community.
- The access to the web services has been reconsidered: While configuring a job as a web service the user gets much more freedom to define the requested web service: The responsibility of using a given web service has been transferred from the portal administrator to the common user.

- The revision of the user interface has been started. As the beginning of this process the colors of the menus has been changed, and the appearance of the menus referring the workflow and job configuration have been slightly modified. However the basic functionality has been retained.

Release Notes to Version 3.3

The version 3.3 is a historic milestone in the development of the WS-PGRADE/gUSE infrastructure. The most important changes are:

- The portlet structure has been reconsidered (see Chapter 4.2) and extended such a way that Administrator user can online inspect and trim the distributed gUSE infrastructure with special emphasis on handling of remote computational resources. Parallel to the changes above the duties of ordinary users to find the necessary computational resources have been substantially eased.
- On the WS-PGRADE front end the obsolete Gridsphere has been replaced by technology leader Liferay portlet container ensuring a much better user experience, reliability, efficiency and easy access to the evolving set of developed portlets of the Liferay community.
- On the gUSE backend new kind of resources has been included in the palette of middleware technologies: According to the paradigm "Computing as a Service" new upcoming technologies as Google Application Engine, and –in the near future - Cloud computing can be included beside the rather traditional Web Service and GEMLCA support, not forgetting the gLite support where by the modification of job monitoring the inter job delay time has been reduced dramatically. By the way all cooperating components of the gUSE has been checked, stabilized and optimized in order to meet scalability needs.

Details on the user side:

- Liferay based WS-PGRADE – JSR 168 GS changed to JSR 286 Liferay portlet container.
- Optimization of the submitter status updates – The more effective and well-documented concurrency API is being used in order to reduce the used resources.
- New portlet: Internal Services – This is made for configuring gUSE services. Existing service properties can be set or modified, new services can be added, connections between components can be defined, properties can be imported between existing components and the whole system configuration can be downloaded. Texts on the UI are jstl:fmt based with multi lingual support. So the website localization can be much easier.
- New portlet: Resources – It is for the management of the available resources which could be run. To the supported middleware, resources and resource details can be defined through a special input environment. The portlet uses the opportunities of the new resource service. Texts on the UI are *jstl:fmt* -based which provide multi lingual support so the website localization can be much easier.
- New portlet: gLite Explorer – It gives a chart to the users for configured gLite VOs which contains the details and services of them. The portlet uses the opportunities of the new resource service.

Texts on the UI are *jstl:fmt* based which provide multi lingual support so the website localization can be much easier.

- GAE Cloud support – Google Cloud became a new supported middleware. For that, new configuration interface and a new plugin had been added to the submitter.
- Configuration interface had been improved.
- New portlet: Public key - The support of remote resources which need dedicated user accounts and SSH level identification has been modified.
- Unauthorized file access blocked – Until now the file access went through the web browser without authentication. In this version Liferay uses its own authentication service to make file access safer and only accessible to the entitled users.
- XSS extinguished – Now our own portlets are protected against malicious HTML and JS inputs.

Details on the administrator side:

- WS-PGRADE can be installed as any custom names – Before that, only "*portal30*" name was allowed, from now on anything can be chosen as the name of the web application.
- WS-PGRADE functions are not available until the services are not initialized – From this release, WS-PGRADE is capable of sensing the available IS connection and until this connection is have not been made yet and all of the portlets will give an error message.
- Upgrade of the outdated Tomcat from 5.5.17 to Tomcat 6.0.29 which is actually the newest available stable version.
- Global configuration center for every service – The new resource manager service is realized by information web application with JPA (openJPA) database management. So the installed services can access the configured resources without problems even from different machines.
- Service administration from the web – Service data and properties stored in database instead of static XMLs and property files, which was the former solution. The database handling based on JPA (OpenJPA).
- Texts storage in database – Instead of storing texts in XML files and in the database as formerly used to be, the xml file was removed, and only database storage is used.
- Expansion of the 1:n service connections – In one copy of gUSE the storage and the WiFi were capable of communication only with one surface/service, this restriction is dissolved and there is no restriction to the number of service connections.
- Creation of web archives – All of the gUSE services and interfaces can be installed as standard web archives, and also they can be deployed into any sufficient web containers.

Restrictions/known bugs:

- The instances of called workflows will not be cleared, just stopped after the eventual suspension of a caller workflow. However the rescue operation is not endangered: A new instance of all embedded calls will be created.

- For the time being embedded workflows may return only single files (not PS collections) on their output ports for the caller workflow i.e. embedded workflows may not serve as abstract generators.
- The propagation of the event that a job instance may not be executed (due to a user defined port condition or due to a permanent run time error) may be erroneous in some (workflow graph dependent) cases and therefore an eventual subsequent collector job may not recognize that the job must be executed using just a restricted number of inputs, i.e. the collector job in such situation waits infinitely for rest inputs which never come.
- The notification of user about the change of job states may clog in case of extreme load of the gUSE system. However the elaboration of workflow is done: The workflow state is "finished" but some job states are not in final state.
- Extreme size workflows may block the workflow interpreter.
- Input port conditions for jobs calling embedded workflows are not evaluated.

Release Notes to Version 3.2.2

Improvements: PBS Support: The Portal is able to serve PBS type resources.

Release Notes to Version 3.2

Improvements:

1. Stability of workflow interpreter has been increased.
2. New paging and sorting method at the display of job instances.

Known bugs:

1. Generator output ports (and the ports which may be associated with more than one file as a consequence of the effect of Generators) in embedded workflows may not be connected to the output ports of the caller.
2. Conditional job call operations at certain graph positions may prohibit the call of a subsequent collector job.

Release Notes to Version 3.1

Limitations of usage of the WS P-Grade Portal due to the temporary shortcomings of the current implementation:

1. The numbers of job instances needed in the case of a Parameter Sweep workflow submission are calculated in a static way during the preparation of the whole workflow submission. Dynamic PS invocation is possible but in this case an upper estimation is needed for the number of PS runs. Let’s assume that the upper estimation given by the user is N and the actual dynamic number of runs is M where M<N. In this case gUSE generates N-M dummy jobs that are thrown away during the execution.

2. If there is a collector job and any of its direct predecessor job instances has the state "init" then the collector will not be executed and the associated workflow instance will not reach the state "finished". It may be a bug because in the case of the "semi dynamic PS" (where M is less than N) in N-M cases no output files will be forwarded to the subsequent job instances, and the state of such job instances will be "no input" by definition. However the state of successors of "no_input" job instances are set as "init" for the time being, so the information will be forwarded to the collector that it needs not to wait for an input further which will never come. The solution will be that the state "no_input" will be propagated to the collector which may run if all expected genuine inputs has been produced. (Please note, that this limitation does not exist more since Version 3.1b6)
3. A similar problem is that the programmed "no_input" cases (and job states) are not distinguished from that when a job does not receives input due to missing configuration or due to network error.
4. There are reported cases when the rescue operation after the suspending of a PS workflow does not restart all needed job instances.
5. The implementation of Template definition is rather "unintelligent": Only the explicitly defined features closeness can be reverted, but not all possible attributes of a job. Up to now the system is not able to handle logical consequences among the closed-open state of attributes: For example if the current submitter is gLite and the user opens the Type field in order to allow other kind of submitters the sub features belonging to the other kind submitters cannot be opened, so there is no way to configure them.
6. For the time being deleting of an Application does not includes the deletion of the eventual instances of embedded workflows called from the given Application.
7. The graphic visualization (time space diagram of job instances) contains a bug in the parameter sweep case: not all job instances are displayed the connection of them may be scrambled.
8. The input and the workflow configuration of a downloaded workflow instance does not correspond to the output in all cases (See warning in 3.7.2.2.1)
9. Embedded workflows can be called from PS workflow with the temporary restriction that the embedded workflows may not contain such a graph path where a generator object is not closed by a collector, i.e. a single set of workflow instance inputs must produce a single set of outputs and not an array of them. A generator object in this context may be a job with generator output port or a caller job which returns more than one files at a given output port upon a single embedded workflow instance invocation. If the user does not comply with this limitation the result is not guaranteed. (See the typical use cases)
10. The number of input files may be forwarded to a job instance of a job having a Collector port is restricted in 30. It is due to the limitation of the EGEE imposed on the number of files may be collected in the input sandbox of a JDL file. As the storage size of the input sandbox is limited anyhow the user is advised to use remote files if the number of input files of a collector port may exceed the value 30.

I. Main Part

Introduction

The WS-PGRADE Portal is a web based front end of the gUSE infrastructure. It supports development and submission of distributed applications executed on the computational resources of the Grid and other DCIs. The resources of the *Grid* are connected to the gUSE by a single point back end, the DCI Bridge.

According our vocation: "The Portal is within reach of anyone from anywhere"

The development and execution features have been separated and suited to the different expectations of the following two user groups:

- The common user (sometimes referenced as "end user") needs only a restricted manipulation possibility. He/she wants to get the application "off the shelf", to trim it and submit it with minimal effort.
- The full power (developer) user wants to build and to tailor the application to be as comfortable as possible for the common user. Reusability is important as well.

The recently introduced public Repository is the interface between the common and the developer user. The developer user can put the ready to run applications in the Repository and the common user can get the applications out from it.

The DAG workflow - based on the successful concept of the original P-Grade Portal - has been substantially enlarged with the new features of the gUSE:

1. Job-wise parameterization gives a flexible and computing efficient way of parameter sweep (PS) applications, permitting the submissions of different jobs in different numbers within the same workflow.
2. The separation of Workflows and Workflows Instances permits easy tracking of what's going on and archiving different submission histories of the same Workflow.
3. Moreover, Workflow Instances – objects created by submitting their workflow - make it easy to call (even recursively) a workflow from a job of the same or of another workflow.
4. The data driven flow control of a workflow execution has been extended. The user can define programmed, runtime investigation of file contents on job input ports.
5. The range of possible tasks enveloped in the unique jobs of the workflows has been widely enlarged by the possibility to call workflows (discussed above) and by the ability to call remote Web services as well.
6. Beyond the manual submission of a workflow, time scheduled and foreign system’s event awaiting workflow execution can be set on the user interface of the WS Portal.
7. The back end infrastructure of the gUSE supports an extended usage: With the help of the DCI-Bridge the Administrator can reach new kind of resources, and the users (developers and common users) may reach them the traditional way.

8. The WS-PGRADE Portal and the back end gUSE infrastructure is not a monolithic program running on a single host but a lose collection of web services with reliable, tested interfaces. So the system supports high level of distributed deployment and a high level of scalability (See details in Chapter 5).

The target audience of the current manual is the developer user and the System Administrator (Chapter 5, 6, 7, and 10).

The structure of the first 3 chapters of the main part of the manual follows the basic development cycle of a workflow:

- In Chapter 1 the static skeleton of a workflow is discussed, describing the Graph and the associated Graph Editor to produce it.
- Chapter 2 describes the concept of Jobs and the rather complicated configuration of jobs.
- In this chapter the parameter sweep related features, job configuration and tightly connected job execution is discussed.
- Chapter 3 discusses the Workflow related issues. It introduces the following terms:
    - The Workflow Instance (the running object created upon Workflow submission)
    - The Template, a collection of metadata, by means the reusability of a Workflow is enhanced
    - The Application, a reliable, tested, self-containing collection of related Workflows
    - The Project, which is the intermediate state of an Application
    - The public Repository where the applications, which can be published, are stored
    - Beyond that, this chapter discusses workflow submission, observation and management related features, strictly separating developer's and common user's methods.
- Chapter 4 gives an overview of the portlet structure of the WS-PGRADE.
- Chapter 5 defines the internal organization of the gUSE infrastructure.
- Chapter 6 introduces the middleware technologies, used in the reachable computational resources. This chapter describes the view mode of the DCI Bridge.
- Chapter 7 defines the central user storage quota management
- Chapter 8 deals with an independent look up system for SHIWA resources.
- Chapter 9 describes the experimental implementation of WFI monitor by which one of the central gUSE components, the workflow interpreter can be monitored.
- Appendix I attached to the main part contains the user interface oriented "On-line Manual" describing the unique menus.
- Chapter 10 describes the Certificates menu.
- Chapter 11 introduces the usage statistics portlet that is represents the collection and visualization of usage statistics in gUSE/WS-PGRADE is responsible for collecting and storing metrics in the database and for display of these metrics.
- Chapter 12 describes the whole steps of user management process: from user account creating to password changing.
- The basic terms and the connecting activities associated to them are summarized in Appendix II

- The Appendix III is a case study i.e. it is a jump start for inpatient users.
- The Appendix IV is a simple case study about the data driven call order of PS jobs.

The goal of the main part is to give a concept based description of the system. The Online Manual (Appendix I) gives a keyhole view: the pages describe the local functionality of the given portlet or form.

1. Graph

The **Directed Acyclic Graph (DAG)** is the static skeleton of a workflow. (See Appendix: Graph Menu)

The nodes of the graph, named jobs denote the activities, which envelop insulated computations. Each job must have a Job Name. Job names are unique within a given workflow. The job computations communicate with other jobs of the workflow through job owned input and output ports. An output port of a job connected with an input port of a different job is called channel. Channels are directed edges of a graph, directed from the output ports towards the input ports.

A single port must be either an input, or an output port of a given job.

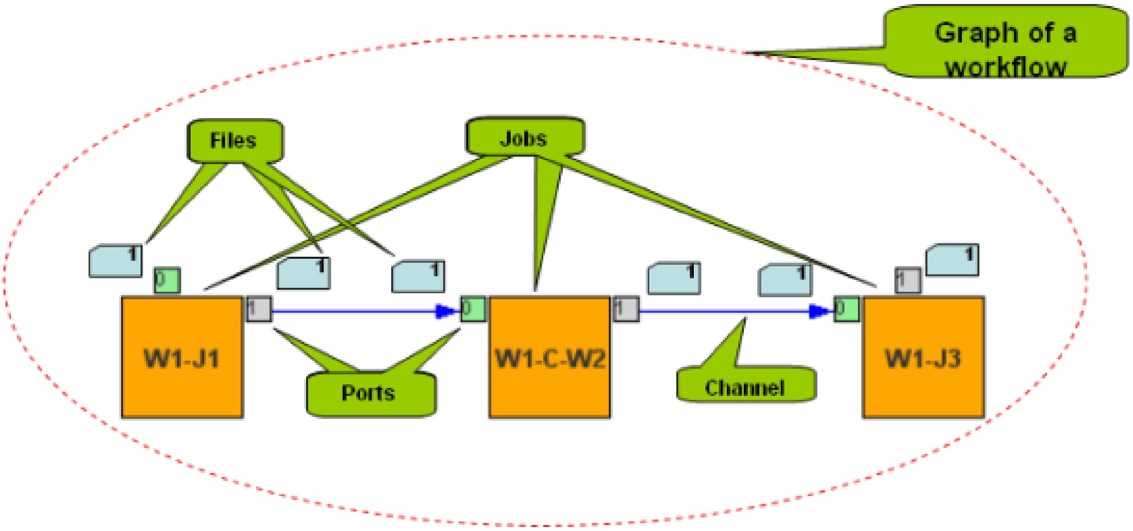


Figure 1 Graph of a workflow

Ports are associated with files. Each port must have a Port Name. Port names are unique within a given Job.

The Port Names serve as default values to the "Internal File Names". The Internal File Names connect the referenced files to the "Open" like instructions issued in the code of the algorithm, which implements the function of the job.

The Internal File Names can be redefined during the Job Port Configuration phase of the Workflow Configuration. (*Workflow/Concrete* tab->*Configure* button of the selected workflow -> selection of actual job ->*Job Inputs and Outputs* tab)

Please note, that presently the Port Names must be composed of alphanumerical characters, extended with "." and "-" characters.

There are immutable port numbers for the physical identification of ports. They are referenced as "*Job Relative Seq*" within the *Graph Editor*. Input ports, which are not channels, i.e. no output port is connected to them, are called genuine input ports. Output ports, which are not channels, i.e. no input port is connected to them, are called genuine output ports.

1.1 The Acyclic Behavior of the Graph

The evaluation of a workflow follows the structure of the associated Graph: The Graph is acyclic, in order to avoid reaching the starting job from any job, including the starting job itself. This acyclic behavior determines the execution semantics of the workflow, to which the given Graph is associated to: The jobs, which have no input dependencies can be executed subsequently, if all their input ports are "filled" with correct values.

1.2 The Graph Editor

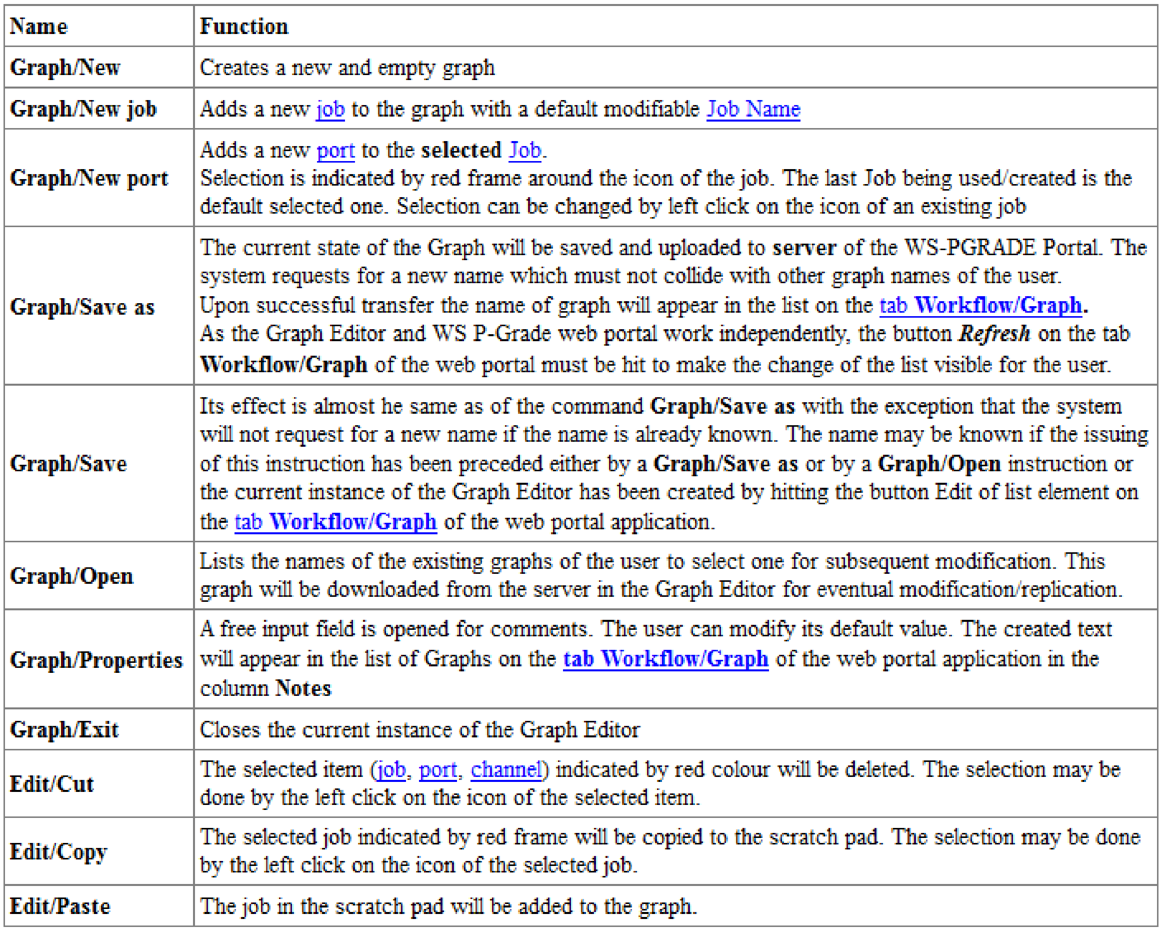
Graphs can be created with the interactive, graphic Graph Editor. The Graph Editor can be reached in the tab *Workflow/Graph*.

Pressing the *Graph Editor* button: a new instance of the Graph Editor can be downloaded from the server of the WS-PGRADE Portal. (See Appendix Figure 2 - Graph Editor) An alternative way to start the Graph Editor is pressing the button Edit, associated to each element of the list, showing the existing user's Graphs. The editor runs as an independent *Webstart* application on the user's client machine.

With the Graph Editor the user can create, modify and save a graph in an animated, graphic way. The Editor can be handled by the menu items or by the pop up menu commands, appearing after a right click on the graphic icons of jobs, ports or edges (channels). (See Appendix Figure 2 Graph Editor) The taskbar containing the icons "Job", "Port" and "Delete" gives an alternative to create jobs, ports (of a selected job) or to delete a selected job, a port, or a channel.

With the slider, the user can zoom in/out the image of the created workflow. The recently touched object (created or identified by left click) becomes "selected". The selected state is distinguished by a red frame around the icon's graphic image. A special - third - editing mode is required for the creation of edges (channels).

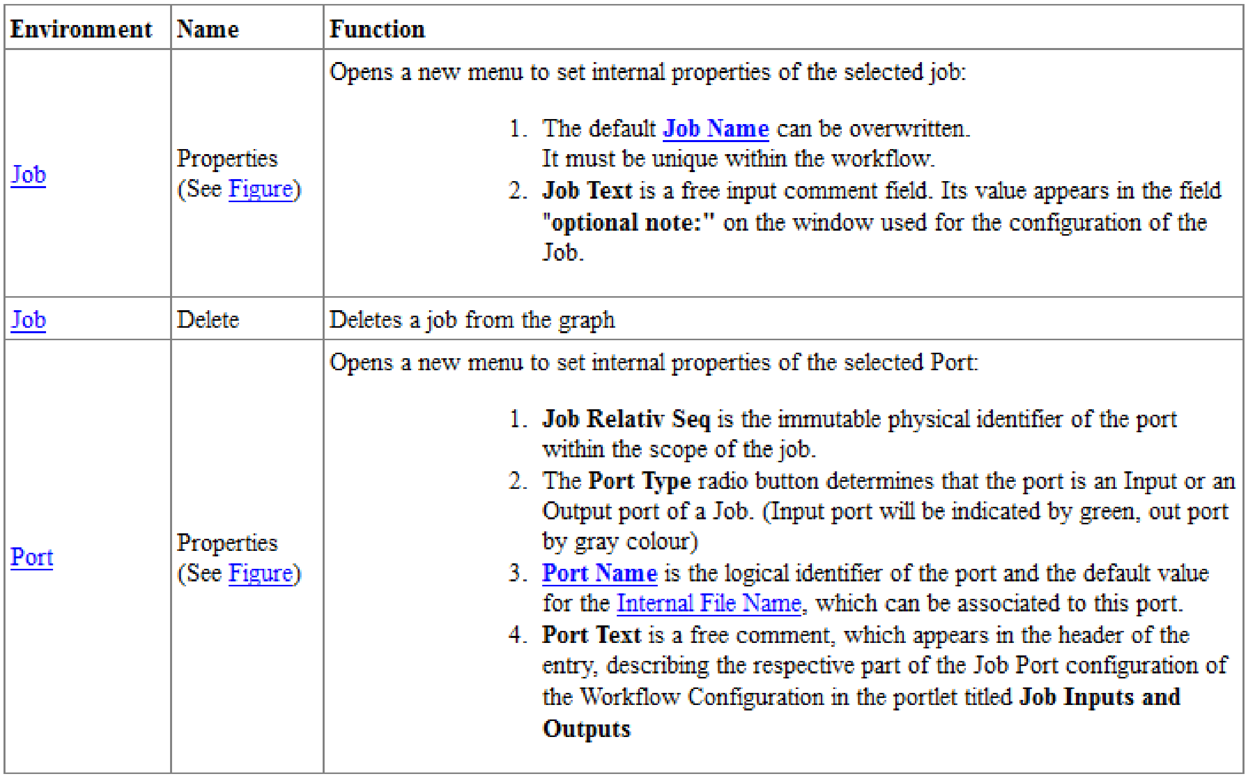
1.2.1 Menu items



Name	**Function**
Graph/New	Creates a new and empty graph
Graph/New job	Adds a new job to the graph with a default modifiable Job Name
Graph/New port	Adds a new port to the **selected** Job. Selection is indicated by red frame around the icon of the job. The last Job being used/created is the default selected one. Selection can be changed by left click on the icon of an existing job
Graph/Save as	The current state of the Graph will be saved and uploaded to **server** of the WS-PGRADE Portal. The system requests for a new name which must not collide with other graph names of the user. Upon successful transfer the name of graph will appear in the list on the tab **Workflow/Graph.** As the Graph Editor and WS P-Grade web portal work independently, the button ***Refresh*** on the tab **Workflow/Graph** of the web portal must be hit to make the change of the list visible for the user.
Graph/Save	Its effect is almost he same as of the command **Graph/Save as** with the exception that the system will not request for a new name if the name is already known. The name may be known if the issuing of this instruction has been preceded either by a **Graph/Save as** or by a **Graph/Open** instruction or the current instance of the Graph Editor has been created by hitting the button Edit of list element on the tab **Workflow/Graph** of the web portal application.
Graph/Open	Lists the names of the existing graphs of the user to select one for subsequent modification. This graph will be downloaded from the server in the Graph Editor for eventual modification/replication.
Graph/Properties	A free input field is opened for comments. The user can modify its default value. The created text will appear in the list of Graphs on the **tab Workflow/Graph** of the web portal application in the column **Notes**
Graph/Exit	Closes the current instance of the Graph Editor
Edit/Cut	The selected item (job, port, channel) indicated by red colour will be deleted. The selection may be done by the left click on the icon of the selected item.
Edit/Copy	The selected job indicated by red frame will be copied to the scratch pad. The selection may be done by the left click on the icon of the selected job.
Edit/Paste	The job in the scratch pad will be added to the graph.

1.2.2 Popup menu items

The popup menu appeared after click on right mouse button.



Environment	**Name**	**Function**
Job	Properties (See Figure)	Opens a new menu to set internal properties of the selected job: 1. The default **Job Name** can be overwritten. It must be unique within the workflow. 2. **Job Text** is a free input comment field. Its value appears in the field **"optional note:"** on the window used for the configuration of the Job.
Job	Delete	Deletes a job from the graph
Port	Properties (See Figure)	Opens a new menu to set internal properties of the selected Port: 1. **Job Relativ Seq** is the immutable physical identifier of the port within the scope of the job. 2. The **Port Type** radio button determines that the port is an Input or an Output port of a Job. (Input port will be indicated by green, out port by gray colour) 3. **Port Name** is the logical identifier of the port and the default value for the Internal File Name, which can be associated to this port. 4. **Port Text** is a free comment, which appears in the header of the entry, describing the respective part of the Job Port configuration of the Workflow Configuration in the portlet titled **Job Inputs and Outputs**

1.2.3 Creation of channels

It is executed in three steps:

1. Pressing the left mouse button over a port icon.
2. Dragging the pressed mouse to a different port icon of a different job.
3. Releasing the mouse button.

Note: The syntax rules are controlled: input port can be associated only to an output port, no destination (input port) of a channel can be shared with different channels, the acyclic property of the graph must be preserved.

2. Jobs

Introduction

The workflow is a configured graph of jobs i.e. it is an extension of the graph with attributes, where the configuration is grouped by Jobs.

This chapter discusses the properties and configuration of jobs. The properties of jobs reflect the elaboration of the enclosing workflow. However the properties of the workflows as a single entity are discussed in Chapter 3. The Job configuration includes:

- algorithm configuration,
- resource configuration and
- port configuration.

The algorithm configuration determines the functionality of the job, the resource configuration determines where this activity will be executed, and the port configuration determines what the input data of the activity are and how the result(s) will be forwarded to the user or to other jobs as inputs. A job may be executed if there is a proper data (or dataset in case of a collector port) at each of its input ports and there is no prohibiting programmed condition excluding the execution of the job. If datasets (more than one data items – where data item is generally a single file) arrive to the input(s) of a job they may trigger the multiplied execution of the job. Exact rules of such – so called parameter sweep (PS) - job invocations will be discussed in chapter 2.3.2.4. At each job execution a runtime environment will be created. It includes the input data triggering the job execution, the state variables and the created outputs. The name of this runtime environment is the job instance object. During the execution of a single workflow one job instance will be created for each non PS job. The N-fold invocation of a PS job creates N job instances.

The collection of job instances created from the jobs belonging to the workflow during a single workflow submission is called workflow instance.

Note: In case of embedded workflow call the execution of the job which calls the embedded workflow creates a new workflow instance of the called workflow.

2.1 Algorithm

An algorithm of a job may be:

1. a binary program,
2. a call of a Web Service (a distinguished form is the calling services by REST – see chapter 18.) or
3. an invocation of an embedded Workflow.

The configuration (See Appendix_Figure_13) of the algorithm can be selected by any of the tabs of the group Job execution model on the job property window (tab *Workflow/Concrete* -> button *Configure* of the selected workflow -> selection of actual job -> tab *Job Executable*).

2.1.1 Binary Algorithm

In case of a binary program - selected as "Interpretation of Job as Binary" on Appendix Figure 13 - the algorithm

- can be coded in a local file to be delivered to an - eventually remote - resource (with some local input files) and executed there (see 2.1.1.1),
- can be a legacy (SHIWA) code (the Submittable Execution Node - SEN): already waiting for input parameters to be executed on a dedicated remote resource (2.1.1.2).
  More details in chapter 23 within Menu-Oriented Online Help
- can be a BOINC Desktop grid related algorithm, where the user may select one of the prepared executables stored on the "middle tier" (the BOINC Server) of the execution sequence. In this

case the job will be executed on one of the client machines (on the "third tier") of the BOINC Desktop Grid.

- can be similar to the previous option: the user may select a valid executable stored in an application repository (EDGI AR). In this case the job will be executed on one of the client machines (on the "third tier") of the BOINC Desktop Grid as well. (chapter 16). Additionally, the place of executing the selected code can be a cloud infrastructure (CloudBroker: chapter 17).

Note: in case of UNICORE-based job configuration the user can select from two options: the user can use preloaded executable from a tool list or he/she can upload binary code by local browser. (See Appendix_Figure_13, Part F)

2.1.1.1 Travelling binary code

In this case translated binary code is delivered to the destination place (defined by the resource configuration), together with the eventual existing local input files.

The executable binary code references the input and output files in the arguments of its "open" like instructions. These references must be simple file names relative to the working directory of the destination where the executables runs.

The same relative file names must be defined as *Internal FileName*(s) during the port configuration of the respecting job. (*Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> *Job Inputs and Outputs* tab).

The kind of the source code can be:

- Sequential
- Java
- MPI

2.1.1.1.1 Sequential

This kind of code may be compiled from C, C++, FORTRAN, or similar source, may be a script (bash, Csh, PERL, etc.) or may be a special tar ball corresponding the name convention *<any>.app.tgz*. This later case will be dissed in the Tar ball as executable paragraph.
Generally, it requests no special runtime environment.

In the contrary case the runtime code

- either must be present on the requested resource or
- delivered together with the executable as input file of the job or
- needs to be mentioned - in case of gLite resources - in the Requirements part of JDL/RSL

2.1.1.1.1.1 Tar ball as executable

The file *<any>.app.tgz* will be delivered to the destination resource. Subsequently the tar ball will be expanded, and the stage script expects a runnable file named as *<any>* in the root of the local working directory, which can be started.

Let’s assume that the original binary program "intArithmetic.exe" expects two text files "INPUT1" and "INPUT2" to execute a basic arithmetic operation, whose result will be stored in the text file "OUTPUT", where the kind of operation is define by a command line argument: for example "M" for multiplication.

We intend to create such a job which receives just one argument (through a single input port which saves the value in file "INPUT1") and this will be multiplied by 2.

The following shell script will be crated and named *as test.sh: #!/bin/sh*

echo "2" > INPUT2
chmod 777 intArithmetic.exe

./intArithmetic.exe M - This file must be packed together with intArithmetic.exe and must be named as *test.sh.app.tgz*. The importance of the tar ball feature is that the complex run time environment of the runnable code can be transferred to the remote site as one entity if it is useful and applicable, and the user need not bother to associate a separate input port to each needed input file.

2.1.1.1.2 Java

The binary code must be a *.class* or *.jar* file. The associated JVM is stored in a configuration file, which can be set only by the System Administrator. The JVM is resource type dependent, therefore it is stored as part of the Submitter (2.2.1).

After job submission Java class (or JAR) code and code of the Submitter dependent JVM is copied automatically to the destination as well.

2.1.1.1.3 MPI

The binary code must be the compilation of a proper MPI compiler. It is assumed that a corresponding MPI Interpreter is available on the requested destination. As the program may spread on several processors (maximum number of needed processors) must be defined.

If a broker is selected instead of a dedicated site, the automatically generated JDL/RSL entry assures that only a proper site is selected as destination, where the MPI dependent requirements are met (see 2.2.3).

2.1.1.1.4 Configuration

The configuration can be done after selecting the Interpretation of Job as Binary tab as Job execution model on the job property window (Workflow/Concrete tab -> Configure button of the selected workflow -> selection the icon of the actual job -> tab Job Executable). See the result on the Appendix Figure 13.

The choices of the radio button Kind of binary selects the type of the binary code among the set members Sequential, Java, MPI. The field MPI Node Number must be defined only in case of running MPI code (see 2.1.1.1.3). The field *Executable code of binary* identifies the code, which must be uploaded from the local environment of the client (by the *Local* option) to the *Portal*, with the help of the file browser button *Browse*. However, you can choose the *Remote* option if your executable binary is not on your local machine. In this case you need to add properly the URL of executable (about the supported remote protocols see *chapter 14: Defining Remote Executable and Input*).

The field *Parameter* may contain eventual command line parameters expected by the binary code. This parameter will be transferred to the destination site of job execution together with the code of executable. The configuration must be fixed in two subsequent steps:

1. In the current page pressing the button Save.. confirms the settings. However, the settings are saved only on the client's machine at this stage.
2. To synchronize the client's settings with the server's settings the user has to use the button Save on Server. (tab Workflow/Concrete tab-> button Configure of the selected workflow) See Appendix Figure 12.

2.1.1.2 SHIWA code

More details in chapter 23 within Menu-Oriented Online Help.

2.1.2 Web Service (WS) call

In the case when the tab Interpretation of Job as Service of the group Job execution model will be selected the job duty is to call an existing remote Web Service.
It has three parameters:

- Type: Reserved for later use. At present the single selectable value is "web service"
- Service: Defines the URL where this service is available
- Method: Defines a web service method. This method should be defined on the remote machine defined as "Service"

A distinguished form of service call is the REST-base service call (see chapter 18.)

2.1.2.1 Parameter passing

Each service method can have some inputs and one output parameter. They must match the Input and Output ports of the current Job.

In the description of the WDSL file the tag "*parameterOrder*" enumerates the input parameter names of the given method. The external association is based on the enumeration of the input port numbers in an increasing order.

Example: let's suppose, that the given job has the input port set containing port numbers {2,7} and "*parameterOrder*" has the value *param_one param_two*. In that case port 2 is associated to "*param_one*" and port 7 is associated to "*param_two*".

2.1.2.2 Configuration

The configuration can be done after setting Interpretation of Job as Service on the job property window (*Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> tab *Job Executable*). See Appendix Figure 15.

By setting the *Replicate* settings in all Jobs check box the current WS job configuration is copied in all Jobs of the Workflow. All settings on the given page must be confirmed by the *Save* button.

2.1.3 Embedded Workflows

Embedded workflows are full-fledged workflows; their instances can be submitted under the control of a different workflow instance.

The workflow embedding implements the subroutine call paradigm: Any workflow with its genuine input (not participating in channels) and all output ports can be regarded as a subroutine with its input and output parameters. A special type of job can represent the caller of the subroutine.
The parameter passing is therefore represented by copying (redirecting) the respective files.

Not all genuine input and output ports of the called workflow must participated in the parameter passing. However, the input of the called (embedded) workflow must be definite. Either a (file) value must be associated to a genuine input port, or the input port of the caller job should be connected to the genuine input port of the called job.

In a similar way, an output port of a caller job must be connected to an output port of the embedded workflow. The remote grid files, direct values, SQL result sets are excluded from the subroutine call parameter transfer:

- The input ports of the caller job forwarding the "actual parameters" may be associated to channels of local files or uploaded local files but not to remote grid file references.
- Similarly the output ports of caller jobs may by just local files but not remote grid files.
- The eventual original file associations of ports participating in the parameter file transfer in the called (embedded) workflow ("formal parameters") will be overruled by the configuration of the connection i.e. by the configuration the caller job of the caller workflow. The concept of workflow instance makes recursion feasible and the possibility of conditional run time port value evaluation ensures that the recursive call is not infinite. As it was mentioned in the introduction, the workflow instance is an object containing the whole run time state of that workflow, extending the workflow definition by state variables and output files. Workflow instances represent the dynamic memory (stack or hype) needed for recursive subroutine calls. This object is created upon each workflow submission. To enforce a kind of security policy, (similarly to the checking the type and number of actual formal parameter passing), only workflows with Template restriction can be used as callable (embedded) workflows.

Summary: The following steps must be done in the simplest case of an embedded application development cycle:

1. Configure the workflow which is intended to be used as embedded.
2. Test the workflow execution for the needed input values.
3. Make a Template from the workflow
4. Create a genuine embeddable workflow by referencing the Template. (Create by Template)
5. Configure the caller workflow (See detailed in the next chapter). During the configuration, define the name of the genuine embeddable workflow in the caller job. As a part of the configuration of the caller job associate all the input and output port of the caller job to a proper input (respectively output) ports of the embedded workflow.
6. Test the application by submitting the caller workflow

2.1.3.1 Configuration of calling of Embedded Workflows

2.1.3.1.1 Selection of the called workflow

The needed specialized type of job in the caller workflow is distinguished by the tab Interpretation of job as Workflow of the group Job execution model on the Job Configuration page (tab Workflow/Concrete -> Configure button of the selected workflow -> selection of caller job -> Job Executable tab). As the semantic of the embedded workflow is hidden, the only possibility here to select an existing workflow from the list box, which has the "for embedding select a workflow created from a Template label. See Appendix Figure 16

2.1.3.1.2 Parameter passing

The parameter passing is defined from the "viewpoint" of the caller job, i.e. it is defined on the port configuration page of the caller. (Workflow/Concrete tab -> Configure button of the selected workflow -> selection of caller job -> Inputs and Outputs tab)

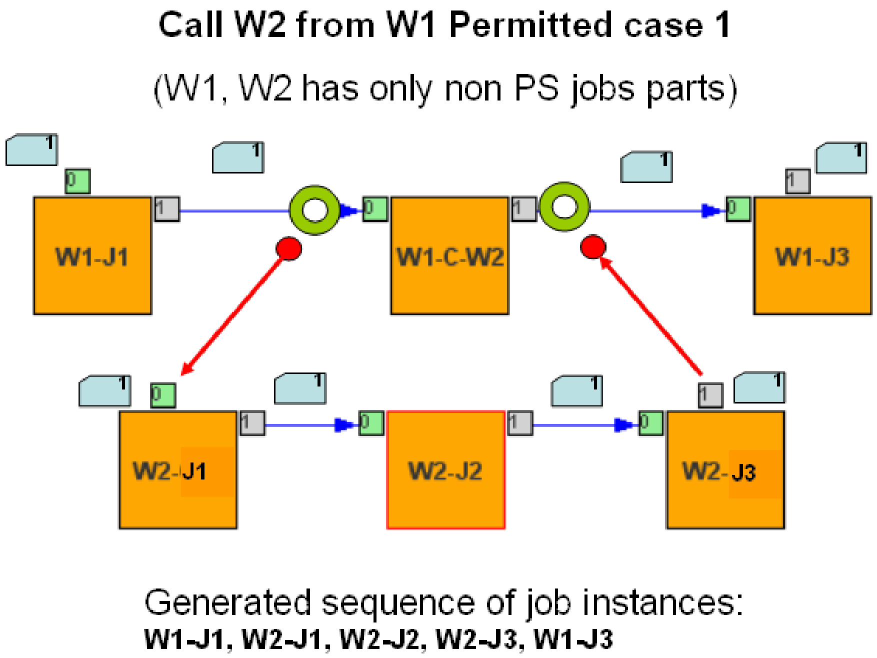
For each port definition, the yes value for the port´s Connect radio button {input|output} port to the Job/{input|output} port of the embedded WF: can be selected.

From the appearing list box Job/{input|output} the proper port of the embedded (called) workflow can be selected.

The list elements can be identified by the string containing the job name and port name, separated by a "/" character. Both names refer to the Graph of the embedded workflow.

Example: See the Appendix Figure 21 for the tab Inputs and Output and the Appendix Figure 22 for detailed explanation.

2.1.3.1.3 Use cases of workflow embedding



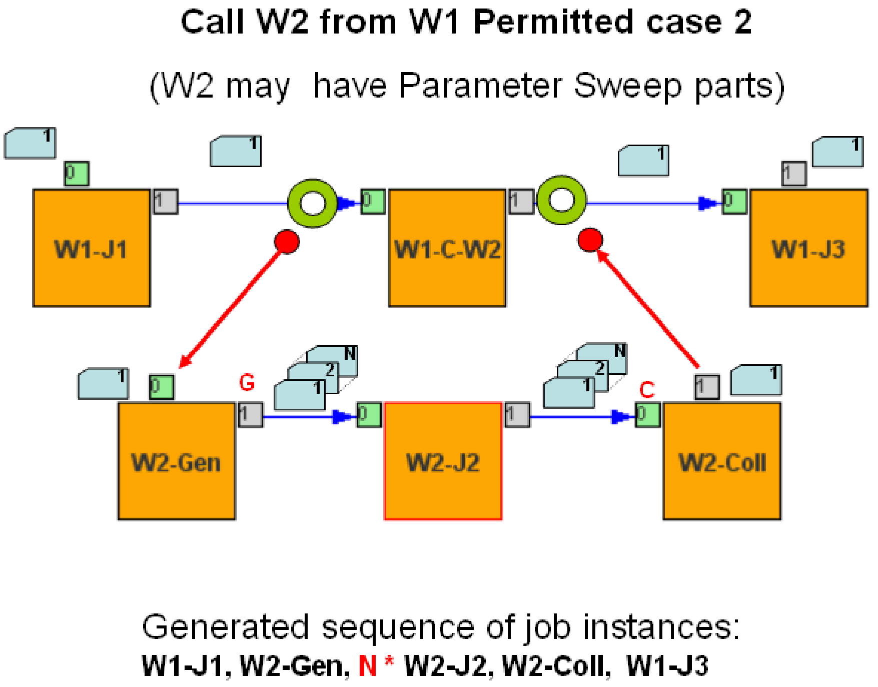
Call W2 from W1 Permitted case 1

(W1, W2 has only non PS jobs parts)

W1-J1
W1-C-W2
W1-J3
W2-J1
W2-J2
W2-J3
0
1

Generated sequence of job instances:
W1-J1, W2-J1, W2-J2, W2-J3, W1-J3

Figure 2 Embedding workflow I.



Call W2 from W1 Permitted case 2

(W2 may have Parameter Sweep parts)

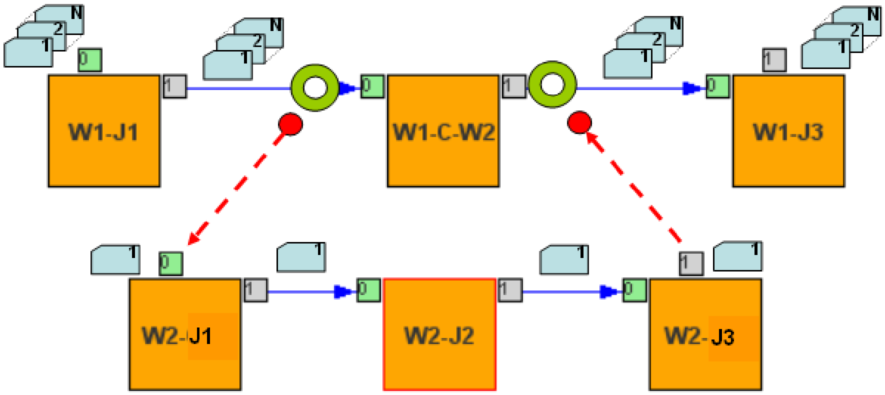
W1-J1
W1-C-W2
W1-J3
G
C
N
2
1
0
W2-Gen
W2-J2
W2-Coll

Generated sequence of job instances:
W1-J1, W2-Gen, N * W2-J2, W2-Coll, W1-J3

Figure 3 Embedding workflow II.

Call W2 from W1 Permitted case 3

(The caller W1 is PS workflow the called W2 is simple)

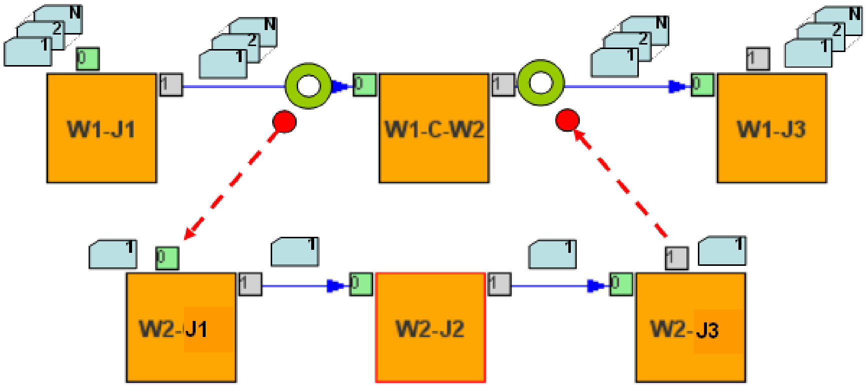

N
2
1
0
W1-J1
1
N
2
1
0
W1-C-W2
1
N
2
1
0
1
N
2
1
W1-J3
1
0
W2-J1
1
1
0
W2-J2
1
1
0
1
1
W2-J3

Intended generation sequence of job instances:
N * (W1-J1, W2-J1, W2-J2, W2-J3, W1-J3)

Figure 4 Embedding workflow III.

Call W2 from W1 Permitted case 3

(The caller W1 is PS workflow the called W2 is simple)


N
2
1
0
W1-J1
1
N
2
1
0
W1-C-W2
1
N
2
1
0
1
N
2
1
W1-J3
1
0
W2-J1
1
1
0
W2-J2
1
1
0
1
1
W2-J3

Intended generation sequence of job instances:
N * (W1-J1, W2-J1, W2-J2, W2-J3, W1-J3)

Figure 5 Embedding workflow IV.

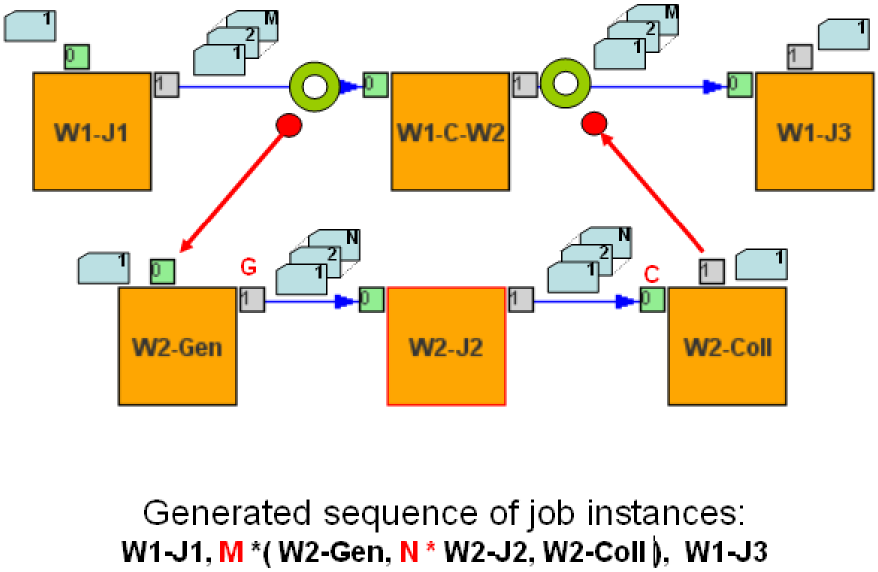
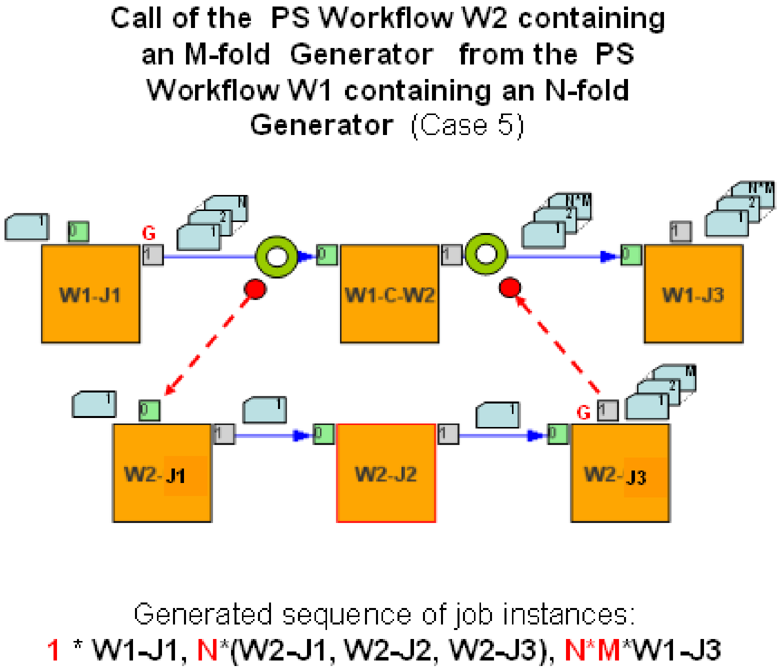
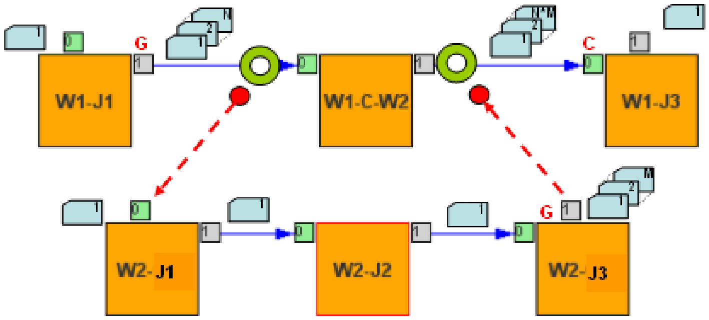

W1-J1
W1-C-W2
W1-J3
W2-Gen
G
W2-J2
C
W2-Coll
M
N
Generated sequence of job instances:
W1-J1, M *(W2-Gen, N * W2-J2, W2-Coll), W1-J3

Figure 6 Embedding workflow V.


Call of the PS Workflow W2 containing an M-fold Generator from the PS Workflow W1 containing an N-fold Generator (Case 5)
W1-J1
G
W1-C-W2
W1-J3
N
N*M
W2- J1
W2-J2
W2- J3
M
Generated sequence of job instances:
1 * W1-J1, N*(W2-J1, W2-J2, W2-J3), N*M*W1-J3

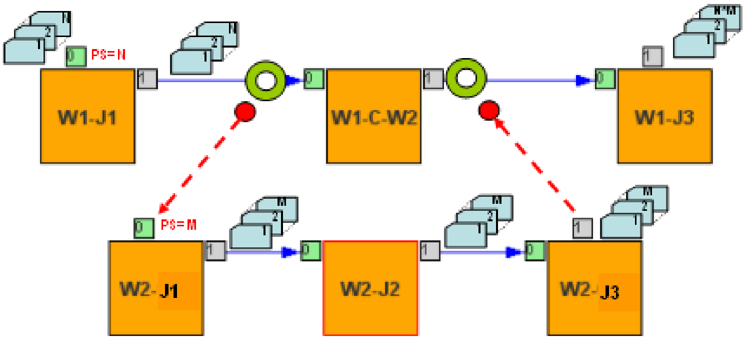
Call of the PS Workflow W2 containing an M-fold Generator from the PS Workflow W1 containing an N-fold Generator and a Collector (Case 6)


W1-J1
G
N
2
1
W1-C-W2
N*M
2
1
C
W1-J3
W2-J1
W2-J2
G
M
2
1
W2-J3

Generated sequence of job instances:
1 * W1-J1, N*(W2-J1, W2-J2, W2-J3), 1*W1-J3

Figure 7a and 7b Embedding workflow VI.

Call of an M size PS W2 from an N size PS (Case 7)


N
2
1
PS=N
W1-J1
N
2
1
W1-C-W2
N*M
2
1
W1-J3
PS=M
W2-J1
M
2
1
W2-J2
M
2
1
W2-J3
M
2
1

This case – that the embedded workflow has a connected PS input - should be avoided as for

$i \varepsilon \{1,2,N\}$; $j = \{1,2,.. M\}$ all $<i,j>$ generations are identical, if the semantics of the w2 jobs are deterministic.

Figure 7c Embedding workflow VII.

2.2 Resource of Job Execution

In our terminology a resource can be any identifiable computing environment, where the algorithm of the job can be executed. For example: a local host, a cluster, a cluster belonging to a Virtual Organization of any Grid, a whole Grid with hidden details, etc. A given resource of job execution - depending on job type and circumstances

- can be defined by the user directly or
- can be determined by the Grid middleware upon the user defined properties of the job.

Broker: In this case the decision may be delegated to the gLite broker. This is the habitual case when the user has access to just a certain Virtual Organization and the broker selects a proper site among the available sites belonging to the given VO.

Important notes:

- The resources in the gUSE environment are set mainly by special property parameters of those Components which are of "*submitter*" type. (See the Internal services menu).
- In cases of certain resource types final parameter setting must be done in the Resources menu.
- In the special case of the PBS resource the user must complete the resource definition using the Public key menu.

If the executable code must be delivered to the resource then – depending on the algorithm and the expectation, about the needed environment of the job execution – the place of the optimal execution can be selected in a hierarchic way defined along the next paragraphs.

2.2.1 Submitter (DCI) type selection

On the top of the hierarchy a submitter type can be selected, where the term submitter refers to a dedicated middleware technology of target DCI, applied to find a resource which has the capacity to match the requirements of the algorithm. There are two kinds of submitters:

1. Local: this means that the system executes the job on a special “local” infrastructure set up and maintained by the local Administrator. It is a dedicated submitter.
2. One of the widely accepted third party middleware technologies which enable the usage of remote resources {GT2, GT4, GT5, gLite, PBS, GAE ..}. Each of them has a dedicated plug in DCI Bridge. DCI Bridge is the unified back end service of the gUSE.

Configuration: the submitter type can be selected by the radio button Type of the job property window (tab *Workflow/Concrete* -> button *Configure of the selected workflow* -> selection of caller job -> tab *Job Executable*). See Appendix Figure 13.

Note: The actual values can be viewed and selected are dependent on the current settings of the *Internal services* menu, which is controlled by the System Administrator of the portal.

2.2.2 VO (Grid) selection

In the one but highest level of resource definition hierarchy a Grid or Virtual Organization (VO) can be selected which supports the selected middleware technology in 2.2.1.

Note: the terms “VO” “Grid” are used with different meanings within the realm of different technologies, and here we use them in a bit sloppy way to indicate the hierarchically highest group of separately administered resources using a common technology.

The proper tabs of the *Resources* menu enumerate the names of administrative domains (Grids/VO-s) using proper submitter (middleware) technology. It is the privilege of the System Administrator to maintain these tables. See the check boxes belonging to the label Grid: on Appendix Figure 13.

2.2.3 Site selection

The site selection may define the place of actual execution of the given job - within the selected administrative domain named VO or Grid (see 2.2.2)
This - third level - selection appears only in the case of certain middleware (GT2, GT4, GT5, PBS, GAE).

Note: In the case of the gLite middleware technology it is assumed that the meta site broker redirects the given job to a proper site suggested by the information system.

To assist the decision of the broker, additional information can be added to the job selected by the JDL/RSL editor. (Choose *Workflow/Concrete* tab -> *Configure* of the selected workflow button -> selection of actual job -> *JDL/RSL* tab).

> Configuration: The site can be selected by the list box Resource: of the job property window. See the part B of Appendix Figure 13. Please note that if the Type is SHIWA then the site and Job manager selection is used in a somewhat different context (More details in chapter 23 within Menu-Oriented Online Help).

2.2.4 Job manager selection

The job manager selection is possible only if the the submitter type (see 2.2.1) is GT2, GT4 or GT5. In the lowest level of the resource definition hierarchy a local submitter (popularly called "job-manager") – in the praxis the name one of a priority queues - can be added to the defined site.

The named priority queues belong to the local scheduler of the cluster which executes the job, where the queues differ from each other in job priority classes. Jobs with high priority are scheduled faster, but their execution time is rather limited, while long jobs will be purged from the system after a longer elapsed wall clock time interval than the high priority ones, but they must run in the background. The information about the local submitters is part of the site definition.

If a site supports more than one job manager than the site must be defined with multiple job manager types in the resource list of the given VO (or Grid). Example: Let us insert (being System Administrator) - by using the New button - the following items on the tab Settings/Resources/gt2 of the selected VO:

(URL= "silyon01.cc.metu.edu.tr", Job Manager ="jobmanager-lcgpbs-seegrid")
(URL= "silyon01.cc.metu.edu.tr", Job Manager ="jobmanager-fork")

(URL= "silyon01.cc.metu.edu.tr", Job Manager ="jobmanager-lcgpbs-seegrid-long")

Configuration: The local submitter of a dedicated site can be selected by the list box Job Manager of the job property window. See the lower part of Appendix Figure 13.For example id the if the selected argument of the list box Resource is silyon01.cc.metu.edu.tr then each of the 3 Job Managers defined in the example above (jobmanager-lcgpbs-seegrid, jobmanager-fork, jobmanager-lcgpbs-seegrid-long) can be selected.

2.3 Port Configuration

Ports associate the inputs and outputs of the insulated activities, hidden by the job with the environment.

2.3.1 Job model dependent access of port values

Values are associated to each input and output ports.
The way these values are connected is different, according to the job model.

2.3.1.1 Case of binary common travelling code

If these values are read/written by binary programs, supplied by the user (See 2.1.1), then the input field Internal file name defines the string, which must be equal with the name of file, which will be opened within the binary program during the run.

This convention makes the transfer of the named values possible. The field *Internal file* name is configurable on the I/O tab. (Workflow/Concrete -> button Configure of the selected workflow -> selection of actual job -> tab Job Inputs and Outputs, see Appendix Figure 16)

Also see Appendix Figure 17 and Appendix Figure 18Shortly speaking, the arguments of the file open like instructions, within the executable, must be associated to the names of local files in the working directory of the resource host, where the executable runs.

- In the input case, the values coming from the port are copied here.
- In the output case, the file, which has the proper Internal file name, is used to forward the values to the output port.

2.3.1.2 Case of binary SHIWA code

More details in chapter 23 within Menu-Oriented Online Help

2.3.1.3 Case of Web Service code

The question of port value passing is discussed in 2.1.2.2.
See Appendix Figure 20 and chapter 2.1.2.

2.3.1.4 Case of Embedded Workflows

The association of ports (caller job to, ports of the workflow) is discussed in 2.1.3.1.2
See Appendix Figure 21 and 22 and chapter 2.1.3 for details.

2.3.2 Input ports

About configuration see Appendix: Figure 17. This chapter deals with the following topics:

- Availability of data to a single port (Port condition 2.3.2.1, Collector port 2.3.2.2)
- Source of data to a single port (Origin 2.3.2.3)
- Effect of data sets received on multiple input ports on the execution of the job (2.3.2.4)

Values to an input port

- may be directly defined values;
- can come from an external source;
- or they can be a file, produced by a foreign job through its own output port.

If each value has arrived on each input ports of a job, then the job can be executed. Two special circumstances may prohibit or postpone the execution of a job:

1. If there is a condition connected to an input port of a job or
2. If it is a collector port

2.3.2.1 Port condition

Pitfall: Port condition defined in the configuration phase to an input port may prohibit the execution of the associated binary or webserver job. (See the restriction notice at 2.6.3.3.1) Optionally, a user can put a condition on the value, delivered by the port.

The run time evaluation of this condition yields a Boolean value. If this value is false, then the workflow interpreter omits the execution of the job and executions of its consequence jobs from the executions. The state of the job will be "*Term_is_false*", when the run time evaluation of the input port condition yields the value false, and the states of eventual successor jobs remain "init". The evaluation of port condition does not influence directly the overall qualification of the state of the workflow: The applied condition is regarded to be a programmed "branch" and the state of the workflow can be "Finished", even if there are jobs remained in "init" and in "Term_is_false" states.

2.3.2.1.1 Port condition configuration

See *Workflow/Concrete* tab -> button *Configure* of the selected workflow -> selection of actual job -> tab *Job Inputs and Outputs*. The choice of value View of the radio button Port dependent condition to let the

Job run: allows the editing of port dependent conditions, to permit/exclude running of the job. In the appearing interface the details of a two argument Boolean operation must be defined:

- The first argument is fixed. It is the value to be delivered by the current port to the job.
- The comparing second argument is selectable by the *{Value: | File:}* radio button allowing to choose the definition of direct comparing Value, or a value of a File received via a different input port.
- In the first case the user defines the direct value in the input field *Value*:, in the second case list box *File*: enumerates the port names to select from.

The kind of the *Boolean* operation must be defined by the list box operation, where one of the

set== (equal);
!= (not equal);

contain. (The first argument contains the second argument if both arguments are regarded as character strings and the second argument is a true substring of the first) can be selected.

Example: The job Job0 may run if the value of the file connected to the port PORT0 has the substring value connected to PORT2. See Appendix Figure 23

2.3.2.2 Collector port

In the base case of Parameter Sweep workflow execution a job within the static context of its workflow (not considering the eventual embedded, recursive cases) receives more than one input files through a given port.

In this case, according to the general rules of port grouping (See dot and cross products at 2.6.1.2.2), each new file participates in a different, new job submission. In the simplest case when a job has just one input port and two files are sent to this port then two job executions (and two job instance creations) will be triggered, one for each file arrival.
However, in case of a Collector Port the job call is postponed, until the latest file is received on this port, and a single job execution elaborates all input files. Because of the special nature of Collector Port there are some restrictions

- on the places where these ports may occur;
- on the name of files they are associated with:

Port occurrence restriction: Because of the nature of collector ports, they can't be genuine input ports which referencing single files. (We call an input port to be genuine input port if it is not the destination of a channel.)
A consequence is that they mustn't be applied in a job encapsulating Web Service, SHIWA or Embedded Workflow call. Restriction on the names of associated files:

- File names must have a fixed syntax i.e. they must contain an index postfix separated from the prefix by an underline character ("_").
- The index must be encountered staring from zero ("0").
- The prefix must match the Input Port's Internal File Name (See 2.1.1.1).

Warning: The usage of the collector ports requires a collaboration of the user defined binary code of the job. It is the responsibility of the user code to find, encounter, and read all the input files whose names match the definition above.

Jobs having the code able to meet these requirements are called as *Collector* jobs.

2.3.2.2.1 Collector port configuration

See *Workflow/Concrete* tab -> *Configure* tab of the selected workflow -> selection of actual job -> *Job Inputs and Outputs* tab. The collector property of an input port can be configured if the radio button is set to *View*. The choice of value All of the radio button Waiting configures a port to be a Collector Port. Example: See Appendix Figure 24.

2.3.2.3 Origin of values associated to an input port

Input ports either can be destination of channels (similar functions have the input ports of embedded workflows, associated to an input port of the calling job) where the received values are defined elsewhere, or the data may be defined at the input port definition (Genuine input port).

2.3.2.3.1 Genuine input ports

Five basic cases are distinguished, each subdivided according to whether a single or a set of files are defined. This latter case is used to drive a sequence of calculations, called **Parameter Sweep (PS)**.
Common, PS related properties of genuine and channel import ports are discussed in 2.3.2.4

Basic sources

Basic data sources of genuine input ports can be:

- Local file
- Remote file
- Direct value
- Online value generation from Database
- Application dependent set of parameters

PS Input Ports: A job may receive more than just one data items via a genuine input port. (See Local, Remote and Database cases). In this cases little integer indices – which are consecutive numbers starting from zero - will be associated to the encountered data items.

But not this but an explicit user defined number (called Input Numbers) associated to the given port determines whether the port will be regarded as a parameter sweep (PS) input port. The default value of Input Numbers is 1 and it means a common Input Port.

If the user redefines it as N > 1, then port becomes a PS Input Port. The number N may differ from the number of existing data items (M). If N < M then the data items encountered by higher indices than (N-1) will be discarded.
If N > M > 0 then additional user defined setting (called Exception at exhausted input) defines what happens if the set of data items of the Basic source is exhausted: Use First means that the data item with index 0 will be reused for all missing indices i where M <= i < N

Use Last means that the data item with index M-1 will be reused for all missing indices i where M <= i < N
Abort means that the job will be aborted and its status will be set as failed. The configuration is shown in the local case on Appendix Figure 25.

Local file

A local file on the client machine is uploaded to the server of the portal, during the configuration phase. Upon job submission the value of this file is forwarded to the resource, where it's elaborated.

Local file configuration

See *Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> *Job Inputs and Outputs* tab. The value *Upload* of the radio button indicating the data source must be selected and subsequently, a local file must be selected by the browser button Browse.. Example: See on Appendix Figure 17 and on Appendix Figure 18 the configuration window before and after the definition of the file to be uploaded. Important note: The appearance of the selected file name in the input field of Upload in itself is not guarantee of the successful upload: As it was emphasized in 2.1.1.1.4 the configuration must be confirmed by the button Save on Server on the workflow configuration window (See Appendix Figure 12)

Special case: In case of REST-type configuration (in channel-type input port at *Stream* as HTTP sending type) the file handling is similar to local file handling (see chapter 18).

Local file configuration in parameter sweep case

In this special case, the name and the content of the file are restricted: The name must be "*paramInputs.zip*" and the content must be a compressed zip file of children files, named as subsequent integers, starting from 0: "0", "1", "2". It is also the responsibility of the user, that contents of the children files are digestible for the job.

See general comments about PS Input ports .Example: See Appendix Figure 25. Notice even if the file "*paramInputs.zip*" contains 10 elements only the first five (indices 0, 1, 2, 3, 4) will be considered.

Remote file

A remote file will not be copied in configuration time, only its way of access is remembered.
The remote storage is visited during job submission time and the proper file content is copied to the destination, where the content is accessible to the job. The URL implementing the access of the remote file is technology dependent:

- It can be LFC Grid file catalogue entry if the Type of the job (See 2.2.1) is gLite or it can be a low level (Globus compatible) one, prefixed with a *gsiftp* protocol. The use of the LFC catalogue does not generate additional duties for the user:
- The proper Environment variables are maintained by the System Administrator in the proper Submitter Configuration File.
- (The Environment variables are needed to assist the system generated scripts to fetch the content of the remote files and put them as local files to the resource, where job is running.)

Note: The WS-PGRADE portal has a special portlet to handle those remote files which use the LFC catalogue technology. (See the LFC menu)

- This portlet is independent from the workflow submission system and supports the user to control the whole life cycle of remote files.

Remote file configuration

See *Workflow/Concrete tab -> Configure button of the selected workflow -> selection of actual job -> Job I/O* tab. The value *Remote* of the radio button indicating the data source must be selected and the associated input field must be filled with the required URL.

Warning: At present, independently of the setting of the check box *Copy to WN* the remote file will be copied to the resource, where the job will run.

The supported protocol list to remote input resource definition is available in the chapter 14.

Remote file configuration in Parameter Sweep case

To get a parameter sweep case the port must be defined as a PS Input Port i.e. Input Numbers must be greater than one.
In this case the user defined URL defined in the input field associated to the radio button selector Remote refers only to the prefix of the paths of files to be accessed. The names of the existing remote files must have an additional postfix, consisting of an underline separator character ("_") and a string of indices starting from 0. It is also the responsibility of the user, that the contents of the remote files are digestible for the job.

Example: The URL *lfn:/grid/gilda/a/b* may refer to the existing grid files
lfn:/grid/gilda/a/b_0;
lfn:/grid/gilda/a/b_1;
lfn:/grid/gilda/a/b_2;

Direct value

In this case, not a file, but a user defined string is forwarded to the job through the port. Differing from the other methods of input definitions, it is not possible in this case to define different contents for subsequent job submissions, if the port is used as PS Input Port. Each PS generation of this port generates a set containing identical files.

Direct value configuration

(See tab *Workflow/Concrete* -> button *Configure* of the selected workflow -> selection of actual job -> tab *Job Inputs and Outputs*).
The content of the input field activated by the selection of Value of the radio button indicating the data source will be delivered as a file to the working directory of the node, executing the job. The name of the file is a user defined one; identical with the input field of Input port's Internal File name.

Online value generation from Database.

The values are generated online (in job submission time) by an SQL Select statement.
Only values are taken from the result set, which belong to the left column listed in the SQL Select statement.

If it has not been defined by the "ORDER BY" clause, the order of elements in the result set is haphazard. In case of simple file generation the first element of the result set is selected to be the content of the input file. At present, only the Unix mysql implementation of SQL is supported.

Database source value configuration

(See tab *Workflow/Concrete* -> button *Configure* of the selected workflow -> selection of actual job -> tab *Job Inputs and Outputs*)
The configuration must be defined in 4 subsequent input steps.
These steps belong to input fields which are hidden until the user selects the choice SQL of the radio button indicating the data source. Example: See Appendix Figure 26.

Database Source

The URL of the database must be defined in the following form:
<LanguageEmbddingProtocol>: <ImplementationProtocol>:// <Host_url> /<path>

Pitfall: At present, only the protocol *jdbc:mysql:* is handled. The input field is labeled as SQL URL (JDBC).

Database Owner

The owner of the file representing the database must be defined.
The input field is labeled as USER.

Database Security

The password known by the owner of the file representing the database must be defined.
The input field is labeled as Password.

Database Query

The argument of the SQL Select statement must be defined.
The input field is labeled as SQL Query SELECT.

Database source value configuration in Parameter Sweep case

From each value of the result set (belonging to the left column of Select statement) a different file will be composed. Example: Appendix Figure 26 discusses the case when the SQL Select statement produces four records but the port is configured as PS Input Port which will receive 10 files.

Application Dependent Parameter Association to a port

It is a special tool to associate input parameters to a distinguished application, which will be prepared by a special –application dependent - submitter, ready to forward these parameters. The tool can be selected by the value "Application specific properties" of the radio button determining the kind of the input. (See Appendix Figure 19)
The button view property window opens a form containing the editable table of required inputs.

Notes: The following additional conditions are needed to use this input definition facility:

The portal administrator makes this option selectable for the user, when the administrator configures the job <*Jobname*> by a special way; by putting the file <*Jobname*>.jsp in the subdirectory named "props", located in a proper place of the Tomcat server.

The file <*Jobname*>.jsp contains the form needed to read the given application specific input parameters, which are forwarded as additional values to the application sensitive submitter of the job.

Shortly speaking, by plugging in the file <*Jobname*>.jsp in the system the control of input definition is passed to the user. It is assumed that the special keys defined in the <*Jobname*>.jsp to identify the parameter, are recognized properly by the special destination submitter of the job.

2.3.2.4 Effect of data sets received on multiple input ports on the execution of the job

A genuine input port may deliver for subsequent job executions more than one files, if the a proper number value is set. This value, called Input Numbers must be defined during the configuration of the job. Its default value is 1 meaning no parameter sweep case. Rules for Input Numbers was discussed in chapter 2.3.2.3.1.1 in the section PS Input PortsIn case of a channel input port, the possibility to set the value of "Input Numbers" mentioned at the genuine input ports is missing, because this number will be computed, and it indicates the overall number of files which must be created on the output of the given channel as a result of the full execution of the workflow. The proper setting of a special additional key (Dot and Cross PID) can connect an input port with other input ports of the same job from the point of view of the parameter sweep controlled job elaboration. See more detailed in 2.6.

2.3.3 Output ports

Output ports describe

- the source,
- destination, and
- lifetime

of data produced by the jobs. Depending on the kind of the job execution model, which may be a binary executable, a service call or the submission of an embedded workflow, the result can be retrieved in a different way.

Note: Special kind of output ports are the **Generator** output ports, where upon the execution of a single job instance more than one file may appear and will be forwarded. (See Appendix Figure 27)

2.3.3.1 Source of output data belonging to the port

2.3.3.1.1 Case of Binary Executable

In case of binary executable code, the source of data is associated to the file whose name is configured by the user in the input field *Output Port's Internal File Name*. See Appendix Figure 27 (tab *Workflow/Concrete* -> button *Configure* of the selected workflow -> selection of actual job -> tab *Job Inputs and Outputs*).

According to the convention made with the author of the binary executable code the user defined string associated with Output Port's Internal File Name must stand in the argument of the "*Open*" like instructions of the Binary executable to determine the location of the generated output file relative to the working directory, on the worker node of the job execution. The same string is used, to define a unique sub library, if the content of the file must be copied to the Portal server as destination.

2.3.3.1.2 Case of Service Call

In case of *Service Call* the proper physical port number identifies the source similar to the case of input ports (see 2.1.2.2)

2.3.3.1.3 Case of embedded Workflow

In case of embedded workflow call, the user must manually select among the possible output ports of the embedded workflow to identify the source.

2.3.3.1.3.1 Configuring the output connection of embedded workflow

See *Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> *Job Inputs and Outputs* tab.

A special form entry is introduced by the "*Connect output port to a Job/Output port of the embedded WF*" radio button. If "*Yes*" is selected then the possible output ports of the embedded workflow appear in the check list Job/Output port:

The method of configuration is identical with that, was discussed in case of the input ports. See further Appendix Figures 21 and 22.

2.3.3.2 Destination of output ports

An output port may define two alternative, basic destinations:

- In one case – remote files -, the result file is stored in the Grid, included and controlled by a so called remote storage.
- In the other case – local files - it can be temporally stored on the Portal Server Machine. It can be downloaded by the user as result, and similarly to the remote case - it can be used as an input of a subsequent job.

Note: In the case of local files, the already mentioned user defined value "*Output Port's Internal File Name*" is used to define and identify the location of the produced file in the file system of the portal server.

2.3.3.2.1 Parameter Sweep behavior

Special consideration is required, if the job producing the output file "runs" several times within the control of the actual submitted workflow instance or when the Job's type is **Generator**, which means that during one job execution it produces more than one file on an output port. As a result of both cases (which may occur together) a predictable number of files can be created on each port. To be able to distinguish these files a postfix index number is added to a common prefix identifier in order to compose a file name. The range of indexing is 0..max-1, where max is the predicted, maximal number of files, which can be generated on that port, during the submission of the given workflow instance. There is a special concatenation character "_", separating prefix identifier from the postfix index. The prefix identifier is destination dependent.

2.3.3.2.2 Remote file destination

In case of remote Grid files the user explicitly defines the name and location of grid files. In case of remote destination the postfix index is added to the file name even in that case when there is no PS behavior. The consequence is that in an eventual Input port definition the file must be referenced by its full extended name (separator + postfix index).The default value of the postfix index is 0.Two cases are possible:

The user may define the remote files within the EGEE infrastructure by high level, symbolic names conforming to the LFN standard for Grid File Catalogues. These names are introduced by the protocol "*lfn*:" following by the hierarchically structured Grid File Catalogue. This catalogue generally rooted as */grid/<VO>/*… where *<VO>* means the virtual organization where the file is maintained.

1. In this case the placement of the file must be defined in an auxiliary line as a Storage Element.
2. In case of low level file access the "gsiftp" protocol is used to define the prefix of the destination URL of the file.

Note: The WS-PGRADE portal has a special portlet to handle those remote files which use the LFC catalogue technology. (See the LFC portlet)

This portlet is independent from the workflow submission system and supports the user to control the whole life cycle of remote files.

2.3.3.2.2.1 Remote file destination configuration

(See tab *Workflow/Concrete* -> button *Configure* of the selected workflow -> selection of actual job -> tab *Job Inputs and Outputs*) See Appendix Figure 27.
The label *Base of Output Port's Remote File Name* introduces input field for the prefix of the destination URL.

Note: The system will extend the name of the created output file by the indexing postfix of form *"_<X> _<Y>"*, where *<X>* is an integer number *>=0* corresponding to the sequence number of job instance which have created the file, and *<Y>* is an integer number *>=0* corresponding to the case that a job instance may produce more than one output file at a given port (certainly only in the case of a Generator job)

The label "SE, if the definition of the remote file has the prefix 'lfn:" introduces an optional filed which must be filled in case of Grid File Catalogue based file name in order to define the URL of the place – in our case of the Storage Element – where the file - more precisely one replica of that – will be stored. Example 1, LFC based, high level definition:

- Base of Output Port's Remote File Name*: lfn:/grid/seegrid/JohnDoe/anyFile*
- SE, if the definition of the remote file has the prefix 'lfn': *se.phy.bg.ac.yu*

The grid file to be created must be referenced by the following Grid File Catalogue name: *lfn:/grid/seegrid/JohnDoe/anyFile_0_0*.

Example 2, low level (GLOBUS 2 based) mapping of a remote file in a local file system:

- Base of Output Port's Remote File Name: gsiftp:/n34.hpcc.sztaki.hu/mass/any
- The grid file to be created will be implemented by a common file named as "any_0_0" in the subdirectory "/mass" of the machine "n34.hpcc.sztaki.hu."

2.3.3.3 Storage type of files generated on the output port

Remote files are regarded to be permanent (as they are saved on external storage devices), but other files - we call them as "local" - must be distinguished: There are channel files, which can be forgotten, after all subsequent jobs have terminated with success. The user can –if he/she is not interested in them- declare them as volatile and they are deleted, after the termination of workflow execution. Consequently these files are not involved in the set of local output files, which can be downloaded as the result of the workflow instance. In the other case - and it is the default one - a local output file is regarded as "permanent" and part of the workflow instance result.

2.3.3.3.1 Configuration of the storage type

(See tab Workflow/Concrete -> button Configure of the selected workflow -> selection of actual job -> tab Job Inputs and Output)
See Appendix Figure 27. The label Storage type introduces the selection between Permanent and Volatile qualifiers.

2.3.3.4 Access to the results produced on the output ports

Permanent Local output files can be accessed in two ways:

1. Either by walking down in the hierarchy of the workflow instances up to the selected job instance to find the button Download file output to reach the file download mechanism of the Internet Browser (See *Workflow/Concrete* tab -> *Details* button of the selected workflow -> selecting the *Details* of the selected workflow instance -> selecting the button *View contents of the selected job instance*),
2. or by using the various possibilities of the Storage menu (See *Workflow/Storage* tab)

Remote files defined by logical names via the LFC can be accessed using the menu File Management.

2.3.3.5 Parameter sweep generator output port

As previously discussed - see 2.3.3.2.1 - jobs producing during a single run more than one file, via a given output port, are called *Generators*. The respective output port is called Generator port. In case of a Generator it is the responsibility of the author of the job’s code to produce such output files in the local working directory of the job’s running environment, which meets the following naming convention for Generator ports:

- They should have the syntax <*FileName*>_<X>,
- where <*FileName*> is identical with the user defined string belonging to Output Port’s Internal File Name and <X> is serial number in range [0..N-1] where N is number of actually generated files.
- The generator property of an output port must be declared during the configuration of the respecting output port.(See the next chapter).
- The executable of the job must follow the <*FileName*>_<X> convention when it produces the names for the generated files.

The consequence is that, if the executable of the job would produce an output file named <*FileName*> and the proper output port would be configured as simple port (not Generator), then the workflow interpreter would not find the file, because the interpreter would seek <*FileName*>_0, <*FileName*>_1 etc.

Name convention of remote output files: The naming convention discussed above has another aspect which may be important for the user in case when remote output files will be generated in PS environment:

- A job J_PS in a PS branch of a workflow may be called m times producing m job instances where each instance may produce n output files on an eventual Generator output port. To store these files the Base of outputs Port's Remote File (see Figure 29) name will be extended by a postfix of form: _<i>_<j>
- where <i> and <j> indicate ASCII code of integer numbers and 0 <= i < m and 0 <= j < n

This extension will be done by the system automatically: The only duty of the author of job's executable to produce the local output files (intended on a generator output) in the form: <*FileName*>_<j>, where <*FileName*> is the Output Port's Internal File Name (see Figure 29). In this case - assuming that the Base of outputs Port's Remote File has the value *<remote>* - the system will produce the remote files with the following file catalogue names: *<remote>*_*<i>*_*<j>*, where i is the automatically allotted index associated to the job instance.

2.3.3.5.1 Configuring a parameter sweep generator output port

See *Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> tab *Job Inputs and Outputs*. See Appendix Figure 27. The setting of the radio button value "*yes*" of "*Generator*" defines a generator port.

The proper output port of a caller job returning a sequence of files (as a consequence of the working of Generator job(s) within the embedded workflow) neither need nor may be configured as Generator because the workflow interpreter recognizes this situation and handles the file sequences properly.

Example: This situation is shown on Figure 5, where the output port of the job W1-C-W2 is not configured as G(enerator).

2.4 Extended Job Specification by JDL/RSL

The modern job submission systems accept job submissions defined by a code written following the rules of a dedicated **Job Description Language (JDL)**. The WS-PGRADE portal liberates the user of the burden to create the syntactically correct JDL code, by composing this code automatically from the user defined job properties. However, advanced users may profit from additional features of given JDL description supported by the selected Submitter. It means, there is not just a single JDL generator built in the portal, but as many, as defined Submitters. Each JDL generator references a separate key file of a common XML type describing keys and types of accepted "ads" in the JDL valid for the given Submitter, where "ad" (abbreviation of advertisement) is the nickname of a key value pair accepted in the given JDL. When the user has selected a resource in a hierarchical way, for the job execution the Submitter has been selected on the height of the hierarchy. The associated key, the XML file is known and the user entering in the JDL/RSL editor, can associate values only to the proper keys (appearing as selectable in the Command list box), which belong to the given submitter.

2.4.1 JDL/RSL description configuration by the generic JDL/RSL editor

See *Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> *JDL/RSL* tab.
See also the online manual about the *JDL/RSL* menu. (See Appendix: Figure28 and 29)
In the *JDL/RSL editor* the user can add or remove "ads". Removing an "ad" happens by the association of an empty string to the selected key. The operation happens in four steps (the first three can be repeated at any time):

1. Select a key by the list box Command
2. Define the associated value in the input text field Value
3. Confirm the defined "ad" by the button Add
4. Confirm all the settings by the button Close

2.5 Job Configuration History

See *Workflow/Concrete* tab -> *Configure* button of the selected workflow -> selection of actual job -> *Job Configuration History* tab.

See also the online manual about the *Job Configuration History*. Job configuration history is a log book, showing the time line of changes performed on the job configuration. *Job Configuration History* must reflect the state of job definition on the portal server. As the Job is configured via the Internet Browser running on the desktop of the user, the Client and Server State must be synchronized. The synchronization point is the save instruction on the workflow configuration level. (See the *Workflow/Concrete* tab -> *Configure* button of the selected workflow -> Save on Server button)

It must be noted, that the History does not shows the preceding configuration steps, if the given job (as part of a Workflow) has been created by a copy of an existing workflow. (See Appendix: Figure 30)

2.6 Job Elaboration within a Workflow

2.6.1 The data driven basic model

The elaboration of the workflows (ordered collection of jobs) follows the next, basically "data driven" model.
See the case study in *Appendix IV*. The example demonstrates the so called "wave front principle" applied in parametric job executions - that each instance of a preceding job elaboration must be completed before any of the instances of a subsequent job would start. This principle must be applied when there is a destination (input) port in the subsequent jobs which has a dot product relation to another input port. (The definition of the dot production assumes that the inputs are paired, and only the wave front principle can ensure deterministic indexing of created output files). Let be noted that this principle is not optimal regarding the throughput of the system, because the execution of a subsequent job – which could have been started must be delayed until all siblings of the predecessor job has terminated. The delay is necessary because the predecessor may have generators, producing unknown number of outputs and therefore the number of output files must be gathered and indexed (named) according strict rules based on the static "pid" values of the generator job instances. The calculated index belonging to an output file calculated by this method will be deterministic and independent of the termination time of the job which has produced the files. We will see later, that there are different ways to influence the order of job submissions.

2.6.1.1 Input side of data driven job elaboration

A common (not PS) job can be called (executed/submitted), if each of its input ports are associated by proper file content and there is no condition (See 2.3.2.1), which prohibits the execution of the job. Certainly, a job can be executed immediately, if it has no input port. Generally, the file content of the respective port (which can be a file(local, or remote); a directly defined string value or the result set of an SQL query as well - in the case of a genuine input port, or the destination of a channel) is connected by the Internal File Name to the code, implementing the job. The only exception is, when the job implements a web service. In this case the sequence of port numbers is associated to the parameter order, defined in the WSDL description of the given service. In the general case, only one file must be associated to an input port to trigger a job submission, the only exception is the case of the Collector port – see later (2.6.3.1.3 Collector control). Summary of job triggering conditions: Availability of all input "file(s)" (One for each common input port/all expected files for Collector Input Ports.)
"True" evaluation of eventual input port conditions. But what happens, if the input side conditions of a job will not fulfill? Even in such cases when all input files (on the genuine input ports) of a workflow are present and the jobs are tested it may occur that a job will not receive the proper inputs because there is

- either a (user programmed) non fulfilled input port condition
- or there is a preceding job which have been aborted.

In parameter sweep cases this situation may be rather inconvenient supposing that we have got finished parallel branches of jobs having produced valuable outputs and a collector job waiting in vain for the result of the failed branch – forever.

To overcome this difficulty a new job state "*propagated cut*" has been introduced: If a job instance does not produces an output then all of successor job instances become "*propagated cut*" – until a collector job occurs. With the help of this "*pseudo*" interpretation of unsuccessful jobs a collector job will know exactly when to start because the preceding job instances must reach either the finished state or any of the no output producing states of error, *term_is_false* or propagated cut.

2.6.1.2 Output side of data driven job elaboration

The elaboration of a job involves the generation of output files on the defined output ports. (Output files are associated to the Internal File Names of the output ports). The output files are created upon the successful termination of the creator job. This means that a job which expects input from a preceding one may not be started (cannot be executed) until the preceding job has terminated successfully.Shortly speaking the execution of the workflow is basically data driven, dictated by the directed channels among the jobs.

2.6.2 States of Job instances

When a workflow will be submitted in a grid states will be associated to the run time implementations of the jobs.
"States" are enumeration constants of the variable state of the object job instance.

There are generic and submitter dependent special job states.
The generic states are the followings:

- *init*
- *submitted*
- *running*
- *finished*
- *error*

- *term_is_false*
- *no_input*
- *propagated cut*

The introduction of the state "*init*" needs explanation as we have stated that states are associated to instances and when a job instance will be created then it will be submitted as well, so its state will be "submitted". The "*init*" state is associated to the fact, that the interpreter calculates the set of all possible job instances in the (load) time of workflow submission i.e. in advance, and the index space (and initial state) of job instances are created statically, during this initialization process. The state changes of a job instance is not as straight forward (submitted -> running -> finished) as in case of workflow instances; depending on the kind of submitter the job can go over and over again through the submitted –> running –> error states several times, without user interaction, as the submitter tries to find a proper resource for the job to run. *Term_is_false* is an exceptional job state, indicating user "programmed" stop against the calculation of a job sequence (See more detailed in 2.3.2.1). *No_input* state is the case when a job instance would receive a non-existing file from a *Generator* job. (See more detailed in 2.3.3.5)

The states of (direct and indirect) successors of jobs which are either *in term_is_false* or *no_input* or *error* states will propagate the state "propagated cut". The workflow instances reaches the (Workflow) Finished state, if there is no job instance in either running, or error or in submitted state, and the states of remaining jobs are either *finished* or *term_is_false* or *no_input* or *"propagated cut"*.

2.6.2.1 Check pointing on the base of job instances

We can summarize, that the workflow interpretation permits a job instance granularity of check pointing, in the case of the main workflow, i.e. a finished state job instance will not be resubmitted during an eventual resume command. However, the situation is a bit worse in case of embedded workflows, as the resume of the main (caller) workflow can involve the total resubmission of the eventual embedded workflows.

2.6.3 Job elaboration detailed

Job elaboration can be subdivided - at least theoretically - in five subsequent activities:

1. Gathering inputs from the defined resources
2. Evaluating input values, if needed (in case of user programmed input port conditions)
3. Making accessible the input values to the execution code implementing job
4. Executing the job and evaluating its success, including the eventual repetition in case of failure
5. Delivering /securing the created outputs of successful executed jobs for subsequent usage

In chapters 2.1 – 2.4 job submissions has been discussed from "configuration of jobs" point of view of. In this chapter some delicate points will be cleared, which are not obvious from the "job as mathematical function" paradigm. Special attention is paid to

- the passing remote files as port values;
- parameter sweep cases when one or more input port will be fed by a set of data forcing a series of job submissions of the current and of eventual subsequent jobs;
- Not purely data driven constructs.

2.6.3.1 Passing of remote files

A file is a remote file, if it is stored and maintained permanently on a dedicated site. The "remote" phrase is comes from the fact, that execution of jobs happens mainly in a computing environment, where the reservation of the computing resource is highly dynamic and therefore the storage of permanent data is not permitted. The storage task is delegated to remotely located hosts, which in the EGEE environment (using the LCG2 and gLite middleware) are called as **Storage Elements (SE)**. Important

Note: The manual handling of the remote files of the EGEE environment is supported in the WS-PGRADE portal by a full featured system - the LFC portlet - which is totally independent from the workflow submission system.

The name **LFC** refers to the traditional name of Grid File Catalogue used in the EGEE to the access these files. The Computing Elements (CE) term is the access abstraction of computing environments, available to the members of a given Virtual Organization to execute jobs of similar types. More precisely a CE is a dedicated queue of a cluster's local submitter. Remote files are either

- low level (for example Globus2) extensions of local files, extended by a URL and by proper – security aware - access protocol (for example *gsiftp*) or
- have a high level service infrastructure, which includes a centralized grid level access and maintenance system, for example LFC catalogues in case of the EGEE based LCG2 and gLite technologies. As these high level grid files can exist in several replicas of the same content scattered in the grid (because of user needs), the common content must not be changed because the synchronized usage may not be ensured otherwise. This has consequences on their usage in the environment of the WS-PGRADE Portal:

The user must be aware that the passing of remote input files –for the time being - is done by an atomic copy. It means that name of the file is passed to the worker node, where the job will run. The content of the remote input file is copied from the storage to the local working directory of the worker node, i.e. the responsibility cannot be passed to the user’s code to perform stream like operations, reading just a fraction of data directly asked from the remote storage. The remote output grid files - whose contents will be created in the working directory of the worker node - will be stored in (eventually replicated) Storage Elements and defined by logical names maintained by the central LFC catalogue system.
The distributed nature of grid files - the Grid File Catalogue is hosted on different machine than the replicas (contents) of files - poses serious data integrity problems, which can be diminishes but not totally eliminated by the use WS-PGRADE Portal. As these files – because their nature - mustn't be overwritten, any job to be executed must make sure - before executing the user’s task - that there is no reference on a grid file with the same logical name to be written. Therefore the job must annihilate - before performing the user defined task - any eventually existing grid file to be written. This may cause difficulties, because of the distributed nature of the grid:

Example: A referenced SE containing the grid file is unavailable and the forced "unregistering" which deletes the name of it from the LFC catalogues causes a permanent storage leak (makes zombie from the given file replica). Remote files may neither be passed directly to embedded workflows nor may be transferred remote outputs of embedded workflows to an output port of a caller job, nor can be defined an output port of a caller job to be remote. Shortly speaking only local files can be exchanged as actual formal parameters at embedded call.

2.6.3.2 Parameter sweep controlled job elaboration

2.6.3.2.1 Introduction to the parameter sweep controlled job elaboration

Parameter sweep regime (where the same job is executed several times fed by the predefined set of input configurations) is one of the most important, basic arguments to use distributed parallel computation, instead of using a single central processor, where the intended computations must be executed in turn. The gUSE infrastructure supports the job level parallelization of the parameter sweep like requests occurring in a workflow. It means, that the user can influence individually how many times a job must run within a given workflow submission. Following the data driven paradigm, the introduction of special ports (Generator port, Collector port) and of special jobs (Generator job, Collector job) enables the parameter sweep – former called as parameter study - (PS) elaboration of a workflow: A single set of input files containing more than one element associated by a port – or several input ports having this feature - may trigger the proper number of submissions of the associated job. The actual number of job submissions and the actual combination of input files is determined by the rules below. Each job submission (execution of the job associated by a single job instance) can produce either a single file in an output port of the given job, or several files in case of a Generator output port (See 2.3.3.5) – composing finally multi element sets in the output ports - which may propagate the PS property to subsequent jobs in turn. It means that the input ports at the destination end of the channels behave as they had been PS input port (See definition below). The only difference is that in case of genuine PS input ports (See 2.3.2.4) the size of set – let's call it "Max Size" (see below) - is defined by user, while in case of ports which become subsequently PS like, it is calculated by the system.

2.6.3.2.1.1 Basic terms: PS Input port, Generator, "Max Size"

Definition: The PS input port (See 2.3.2.4) is a special genuine input port. Its distinguished feature is that more than one file are associated to it.
This association may happen several ways:

- uploaded by a single compressed file hiding the set of files,
- by a Grid File Catalogue pointing on a subdirectory instead of a single file, or
- by a result set of an SQL query

An output port is named Generator port (See 2.3.3.5) if more than one file can be created on it, belonging to it during a single Job submission. Each of the PS input ports has an own number attribute which we will refer here as "Max Size":"Max size" is defined in the case PS input ports as the input field "Input Numbers" (See Appendix Figure 25).

The Max Sizes of the special ports - together with special relations among the input ports of a job which will be discussed later - determines the number of subsequent job submissions within a workflow such a way that all jobs will be fed by all of the prescribed combination of input data. However the effective number of job submissions may be fewer: In case of PS Input Port there may be an exception (and the associated run time job error state *no_input*) if the number of really existing files is less than the "Max Size". (See 2.3.2.3.1.1) The elaboration of the jobs is executed for each - prescribed - combination of file contents of the input ports.

2.6.3.2.1.2 Simple PS example

In a simple case let's assume, that a job J has one PS input port, PI and two output ports PO1 and PO2.
Let us define the semantics of the job by the following two functions, each connected to different output ports:
fo1=J1(fi);
fo2=J2(fi);

Let's assume that the content of PI is {fi0, fi1, fi2} i.e. PI is a PS input port containing three different files.
Because of the data driven principle the PI triggers three subsequent job elaborations with the result that:

PO1 has {fo1_0 = J1(fi0), fo1_1 = J1(fi1), fo1_2 = J1(fi2),} and
PO2 has {fo2_0 = J2(fi0), fo2_1 = J2(fi1), fo2_2 = J2(fi2),} content

2.6.3.2.2 The propagation of PS behavior

If PO1 and/or PO2 of the example above are sources (output ports) of channels for other jobs then the destinations (input ports) of these channels would behave as they would have been PS ports – we will use the term derivate PS ports - , i.e. the data driven PS activity propagates itself through the whole DAG. It should be noted, that in case of these "derivate" PS ports the "inherited Max Size" can be calculated as the number of job submissions at the source of the channel multiplied by the number of produced files on the eventual Generator output port of the channel.

Example: Let's suppose that the Job J has a genuine PS input port with *Max Size = 3 ({fi0, fi1, fi2})* and has a simple output port PO1 connected to job B, and a Generator output port PO2 (producing 4 files in a single run) connected to the job C. Let us define the semantics of the job J by the following two functions, each connected to different output ports:

fo1=J1(fi);

fo2=J2(fi,i);

In this case – if there are no other PS input ports end generators in the workflow – the job B will be submitted 3 times, and the job C 12 times.

- B will receive the input set {fo1_0 = J1(fi0), fo1_1 = J1(fi1), fo1_2 = J1(fi2)}
- C will receive the input set {fo2_0 = J2(fi0,0), fo2_1 = J2(fi0,1), fo2_2 = J2(fi0,2), fo2_3 = J2(fi0,3), fo2_4 = J2(fi1,0), fo2_5 = J2(fi1,1), fo2_6 = J2(fi1,2), fo2_7 = J2(fi2,3), fo2_8 = J2(fi2,0), fo2_9 = J2(fi2,1), fo2_10 = J2(fi2,2), fo2_11 = J2(fi2,3)}

2.6.3.2.3 Number and way of PS job submission in case of multiple input ports

Up to now, we have investigated only the case, when a job has just a single input port for the transmission a set of input files. However a job may have more input ports and in parametric case one or more ports may contain a whole set of input data to feed the job. The user must have a wide range of possibilities to combine the inputs. In order to support the user new relations of input ports has been introduced:

2.6.3.2.3.1 Cross Product Set and Dot Product Group

The terms **Cross Product Set** and **Dot Product Group** are introduced to describe relations of different input ports of a job from the PS generation point of view:

If a job has more than one input ports, which have - directly or indirectly - PS sets associated to them, then these ports need to be grouped in user configured Cross Product Sets (CPS): The files belonging to ports, which are in a common CPS are "fully combined" and inserted in sets called CPS Manifolds: The size of the CPS Manifolds are the multiplication of "Max Size" numbers (original or inherited) of the participating ports, and the members of CPS Manifolds are composed from each possible combinations of files, where the files of a single member are selected from all different involved ports. The term "Cross Product" refers to the habitual operator of "Descartes product" of involved base sets. Important note: A port becomes a member of a CPS if its "Cross and Dot PID" number (See 2.3.2.4) is changed by the user to show on the "*Dot and Cross PID*" number of a different port. (See Appendix Figure 25)

In this case the two ports are mutually related and are belonging to a common CPS. Any not related port can be joined to any existing CPS.

As default - in the beginning of the job configuration - each input port has a different "Dot and Cross PID", i.e. each belongs to a separate – consisting one element - CPS.
The remaining (not unified) CPS sets compose a common, so called "Dot Product Group".
The CPS Manifolds which has the maximal size in the Dot Product Group determines the number of job submissions. There is a common indexing over the range [0..max-1], selecting the subsequent CPS Manifold member in each CPS.
Files belonging to the common index, serve as inputs of the subsequent job submission.
If the system reaches to an index, where in the given CPS the referenced CPS Manifold does not exist (because the set have been exhausted) it is replaced by the first member.

Cross and Dot Product Examples

As an illustration let's extend the Simple PS Example by a successor job B, which has two input ports (B_PI1, B_PI2) and one output port B_PO, in such a way, thatPO1 is connected to B_PI1 and
PO2 is connected to B_PI2

Pure Cross Product Example

Let be cross product relation between *B_PI1* and *B_PI2*.
For example Dot and Cross PID of B_PI1 = 0 and Dot and Cross PID of B_PI2 = 0: In this case, each combination (3x3) induces a separate job submission with the following result:

B_PO={
B(fo1_0, fo2_0), B(fo1_0, fo2_1), B(fo1_0, fo2_2),
B(fo1_1, fo2_0), B(fo1_1, fo2_1), B(fo1_1, fo2_2),
B(fo1_2, fo2_0), B(fo1_2, fo2_1), B(fo1_2, fo2_2)
}

Pure Dot Product Example

Let be a dot product relation between *B_PI1* and *B_PI2*.
For example Dot and Cross PID of B_PI1 = 0 and Dot and Cross PID of B_PI2 = 1: In this case, only the length of the input sets - in our case 3 - separate jobs triggered submissions:
B_PO = { B(fo1_0, fo2_0), B(fo1_1, fo2_1), B(fo1_2, fo2_2) }

Mixed Cross and Dot Product Example

Example: Let's suppose that we have three input ports {P1, P2, P3} with different number of received files

P1{ f11, f12, f13 },
P2{ f21, f22},
P3{ f31, f32, f33, f34 },

where the first and second ports are in cross product relation:
For example Dot and Cross PID of PI1 = 0; Dot and Cross PID of PI2 = 0; Dot and Cross PID of PI2 = 2;:
In this case the following file triplets triggers the job, altogether in 6 times = max (length (P1 x P2), length (P3)) = max(3*2, 4) = 6

(PI1xPI2) o PI3)

{ f11, f21, f31 }; submission 1
{ f11, f22, f32 }; submission 2
{ f12, f21, f33 }; submission 3
{ f12, f22, f34 }; submission 4
{ f13, f21, f31 }; submission 5
{ f13, f22, f31 }; submission 6

Note: When the shorter component CPG list - in our case the four element *P3{ f31, f32, f33, f34 }* – is exhausted then the missing elements in the common input set members will be replaced by the first one of the CPG list in question – marked by Bold.

2.6.3.2.4 Collector control

The logical opposite of the Generator (a job having at least a generator output port) is the special job, which has an input port that expects not one, but the whole sequence of input files, which are ready and available before they are elaborated within a single job submission. (See 2.3.2.2 Collector port) This kind of port is distinguished by a Boolean marking, and it is the responsibility of the program logic implementing, that the job finds and reads all of these input files. Let's conclude this chapter with the following example.

2.6.3.2.4.1 Collector control example

Let be a workflow is of the following structure
G -> J -> C
where G is a generator job producing 5 files on its output, J is a common job and C is a Collector job. It has a Collector input port on the destination side of channel connecting it with job J. Then the job G runs one time, the job J five times, and the job C - waiting for all outputs of J - just one time.

2.6.3.2.5 Summary example of PS generation in a workflow

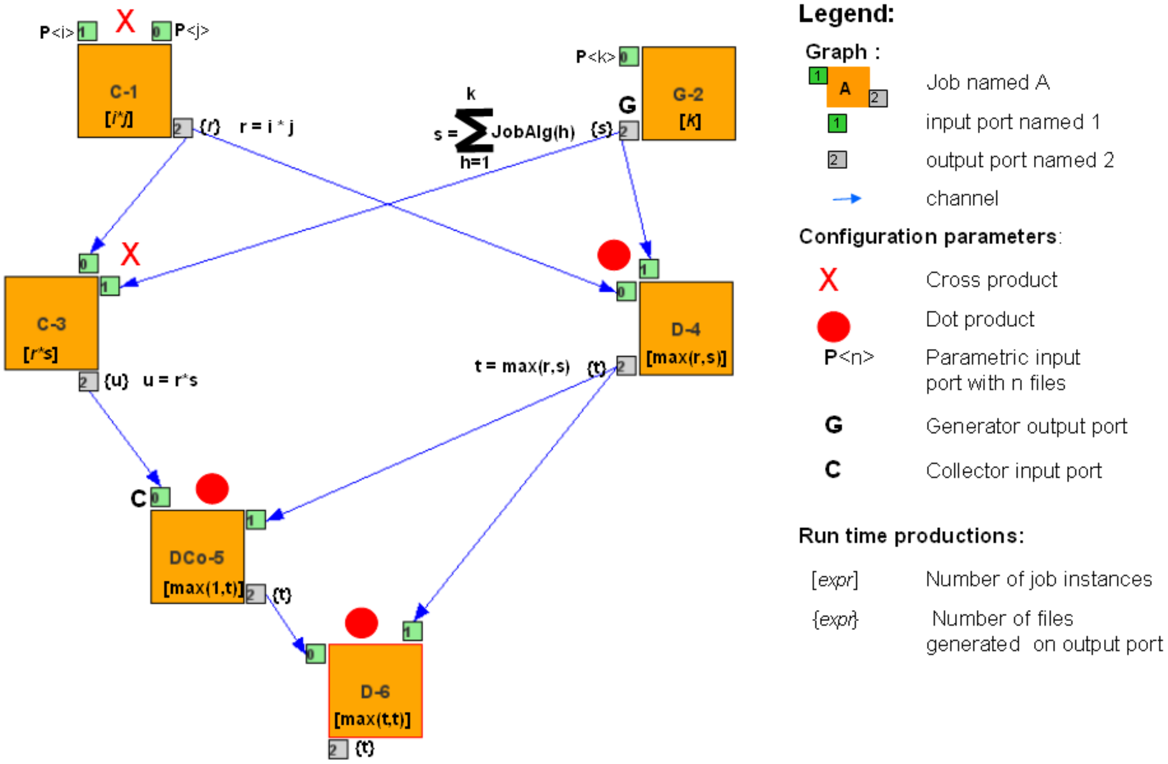

P<i>
X
P<j>
C-1
[i*j]
{r} r = i * j
P<k>
G-2
[k]
G
k
s = ∑ JobAlg(h)
h=1
{s}
X
C-3
[r*s]
{u} u = r*s
D-4
[max(r,s)]
t = max(r,s) {t}
C
DCo-5
[max(1,t)]
{t}
D-6
[max(t,t)]
{t}
Legend:
Graph :
A
Job named A
input port named 1
output port named 2
channel
Configuration parameters:
Cross product
Dot product
P<n>
Parametric input port with n files
G
Generator output port
C
Collector input port
Run time productions:
[expr]
Number of job instances
{expr}
Number of files generated on output port

Figure 8 Example workflow with generator, collector and with ports connected in dot- and cross product relations

Figure 8 demonstrates data driven progress of job elaboration controlled by the gUSE workflow interpreter.

1. It is assumed that the common job “C-1” receives parameter sweep datasets on each input ports, and there is cross product relation among the input ports, which means each element of the given input set must be combined with the members of the other sets participating in the cross product relation. If the production system receives i files on port “1” and j files on port “0” then i*j combination must be calculated i.e. the “C-1” job will be called i*j times and the independent running of i*j job instances will create i*j output files finally. In our terminology a job is common if its algorithm corresponds to the graph representation: In our case it expects two input files and produces a single output. However both of the input ports of C-1 are configured as distinguished parametric input ports, because the job is fed by set of input files and not by single files.
2. The job “C-2” is not common but a generator job. It means that a single run of the job may produce more than one file on one (or more) distinguished, so called generator output port(s) of the job. The number of outputs need not be predictable. In our example this job receives a parametric sweep dataset (via a parametric input port) containing k input files. The k inputs trigger k job executions (k independent job instances) and a not predictable number of output files (see the summarization resulting “s” on the figure...) where each job execution may produce different number of outputs.

3. The Job “C-3” is a common job. It receives aggregated inputs from the preceding jobs. The job will run u*s = i*j*s times because of the cross product relation of its input ports and u*s output files will be created finally.
4. The job “D-4” is a common job as well. However its input ports are in dot product relation. “Dot product” in our terminology means pairing according to the common index of enumerated members of constituent datasets. If the size of one constituent dataset is less than the biggest set involved in the relation, then the missing part of the “pair” will be replaced by the member having the highest index. It follows the example job will be executed either u=i*j or s times depending the value of the max(u,s) function.
5. The job DCo-5 is a collector job. Collector jobs expect no single files but whole data sets on their distinguished collector input port(s). The execution of the job will not start until each expected input file has arrived, and a single job instance will elaborate the whole set. However the example job will be executed *t* times, because its input ports are in dot production relation and the files arrive on input port “1” force the creation of *t* job instances. Each job instance will get the whole u size set of files at the collector port “0” and the next member of *t* size collection arriving at port “1”.
6. The job D-6 is a common job. Its input ports are in dot product relation. The job will be executed *t* times - pairing the inputs of equal sizes - resulting t output files altogether.

2.6.3.3 Not purely data driven elaboration of a workflow

There are three possibilities by which the basic data driven elaboration may be modified:

1. Input port based condition, to submit a given job sequence
2. Call of embedded workflows.
3. By a user or by system induced interrupt.

2.6.3.3.1 Job Input Port based condition

The eventual comparison of a file content, belonging to an input port with a predefined value or with a different input file content yields a Boolean value. The FALSE evaluation on any port subject to the investigation of this kind, excludes the job (and its successors) from the evaluation of the workflow. The state of the job where input port condition has caused the suspension of the execution has a special value: "term_is_false". The state of subsequent jobs will gain the state "propagated cut". The branches excluded such a way from the overall elaboration will not influence the result state of the workflow, i.e. if the elaboration of each job along the permitted branches succeeds, then the overall the state of the workflow is "finished". See also in 2.6.1.1 and in 2.3.2.1Important note: The Job Input Port based condition feature does not exist (and therefore cannot be opened during the configuration of the port) if the port belongs to a job which calls embedded workflows. See next paragraph.

2.6.3.3.2 Call of embedded workflows

The insulated, computational logic hidden behind a single job may be the invocation of an existing, defined workflow of the same user. The input ports of the caller jobs can be associated to certain genuine input ports of the called (embedded) workflow, certain output ports of the called embedded workflow can be associated to the output ports of the caller job, and the mode of evaluation corresponds to the classical subroutine call paradigm. See an example on Appendix Figure 22. Moreover, the call can be explicitly, or implicitly a recursive one as a new Workflow Instance object is created upon the submission of a workflow (storing the intermediate files encoding the run time state and the output files of the workflow). With the common application of the input condition (on job ports) and the application of the recursive embedding, the DAG imposed ban on the repeated call of a job of the workflow can be circumvented. (The other trivial way of bypassing is the Parameter Sweep regime.)However, in the current implementation there are rather strong restrictions, when the embedded workflow call can be used:

- Within a PS environment an embedded workflow - knowing nothing about the number of its proposed invocation - cannot be used safely. The main cause is that, the index space of the PS cases is calculated in a static way, before the invocation of the workflow.
- On the input side, only the passing of the local (uploaded or channel) files are supported, but there is no support for remote files, or of unnamed files, built of direct values, which can be defined during port configuration at common input ports.
- The SQL input can be neither used (which would combine the difficulties mentioned at the PS and the direct value cases).
- On the output side, the local file generated by the embedded workflow cannot be associated to a remote file, defined on the output port of the caller job.
- The ports of the embedded workflow associated to a remote file cannot be involved in parameter passing.
- Only workflows created by Templates can be embedded.

Technically the configuration of embedded workflow call happens in two steps:

1. In the tab Job Executable (tab Workflow/Concrete tab -> WF selected -> Job selected) the choice "Interpretation of job as Workflow" is selected as Job execution model and from the list labeled as "for embedding select a workflow created from a Template:" a proper workflow is selected. (See more detailed in 2.1.3.1.1)
2. In the parallel tab "Job Inputs and Outputs" there is the "Connect input port to a Job/Input port of the embedded WF" option to each input port of the caller job. If the option is selected, then the list of associable input ports of the embedded workflow can be selectable and are showed as Job/Port Name pair. The same is true for the output ports selecting the "Connect output port to a Job/Output port of the embedded WF" option. (See more detailed in 2.1.3.1.2)

2.6.3.3.3 Interrupts and recovery from interrupts

The cases falling in the following categories may prohibit a job run and terminate normally:

1. a user issued interrupt (by the command Suspend)
2. an ill tested workflow configuration or badly programmed job or
3. a network error or not availability or malfunction of a system component

In case 1 the user may resume the workflow's run (job level checkpoint) or delete the run of the whole workflow instance. In cases 2 and 3 the system automatically tries to repeat the execution the failed job several times. If the failed state remains persistent then the successors of the failed job will gain the job state *propagated_cut*. The end state of the workflow instance will be error. However the evaluation along the healthy branches will be continued, even the collectors gathering the files from the healthy and ill-fated branches will be executed – certainly on the existing files reduced in numbers. See also in 2.6.1.1.

3. Workflows and Workflow Instances

A workflow is the description of the call sequence of the involved Jobs (See Chapter 2) belonging to the nodes of a given Graph (See Chapter 1). Shortly speaking a workflow is the semantic description of a complex calculation.

This description includes:

a) Graph description and a
b) set of job descriptions which must include the eventual external sources of genuine input ports.

There are two basic ways to define a Workflow:

1. Developer (alias Full power) User can create it or modify it totally.
2. Inexperienced (alias Common) User can modify only the parts of it permitted by the Developer. In this later case the common user has a simplified, one webpage form to define her parameters instead of configuring each job separately locating it by the Graph.

The full power user has sophisticated tools to support development, reusability, and advertisement of workflows.

A workflow can be submitted when each part of it is defined semantically, and – to meet the authentication and authorization requirements of the grid - there is a valid grid proxy certificate to each resource which will be involved in the calculation.

The submission of the workflows can happen by the following events:

a) The user calls the workflow interactively within the WS-PGRADE Portal (See 3.2.2)
b) A Unix "crontab" like static time scheduler invokes the workflow (See 3.2.3)
c) En external service call triggers the start. (See 3.2.4)

Upon submission a new workflow instance will be created from the workflow.

A workflow instance contains the intermediate (runtime state) variables needed to the control of the workflow and the increasing number of instances related local files.

Warnings: There are several subtle points to discuss here:

The relation of workflow and workflow instance (or job and job instance) is conceptually just the same as the relation of Class and Object in an object oriented formal system i.e. a new instance will be created upon a Workflow submission. So the user may generate any number workflow instances from the same workflow.

The user has the right to redefine the readable external identifier of the workflow instance (the default identifier is date of the submission in case of directly and interactively started workflow.)

The change of a workflow definition in a time interval after the workflow submission and before the termination of the i-th workflow instance have been created from it MAY cause unpredictable changes in the evolution(s) (and result(s)) of the workflow instance(s).

Upon calling a job containing a reference of a workflow, a new workflow instance will be created from this workflow with a generated - unique - external identifier containing the name of the caller Workflow Instance.

The job instance must be distinguished from the job definition: In case of parameter sweep a given number job instances will be created to elaborate the different input sets received by the given job.

The job instance elaboration may create the related local files (log, stdout, stderr, and the local files on the output ports.

Other as the local files, the remote grid output files are referenced by names which are unique in a static common hierarchic name space and the resubmission of a workflow overwrites the ones which have been created by the preceding workflow instance.

The paragraphs of the current chapter are organized as follows:

- Methods of workflow definition (See 3.1)
- Workflow submission (See 3.2)
- Workflow states and Instances (See 3.3)
- Observation of workflow progress (See 3.4)
- Fetching the results (See 3.5)
- Templates for the reusability (See 3.6)
- Maintaining Workflows (See 3.7)

3.1 Methods of Workflow Definition

3.1.1 Methods of workflow definition Introduction

The full power (or developer) user may create, modify, and export workflows. Even generic descriptions can be abstracted from workflow definitions by the full power user:

These abstract descriptions are called *Templates* and they define restrictedly modifiable frames. These frames can be used to define new Workflows with (partly) predefined properties. The inexperienced (common) user has only the right to import a workflow from the registry. Generally these workflows are constrained by a *Template* i.e. only a fraction of the parameters (typically some input files and/or some proper command line parameter of job executables) can be changed by the common user in a simplified user interface.

3.1.2 Operations of a full power user

3.1.2.1 Workflow creation

There are 5 different ways to create a new workflow:

1. Creating an empty workflow (See 3.1.2.1.1)
2. Cloning of an existing Workflow (See 3.1.2.1.2)
3. Using a template to create a new workflow. (See 3.1.2.1.3)
4. Uploading of a previously downloaded workflow (See 3.1.2.1.4)
5. Importing of a previously exported workflow (See 3.1.2.1.5)

Created workflows must have distinguished names in the workflow namespace of the given user. Because historical causes workflows and templates have a common namespace, where name collisions are not permitted. The user can add Notes upon "true" creation (excluding the cases Upload and Import)

3.1.2.1.1 Creating an empty workflow

This operation can be performed by selecting "*Graph*" of the choice "*Create a new workflow from a*" in the tab *Workflow/Create Concrete* (See Appendix: Figure 5)

The associated opening list box encounters the names of available existing graphs to select from. The basic way of creating a new (empty) workflow is performed by associating of an existing graph to it. Let be noted that each of the other four creation methods involves the referencing of a single and just a single graph. Since the time a graph has been bound to a Workflow (or involved indirectly in the definition of a *Template*) the graph cannot be changed. That means that before modifying or deleting a bound Graph each dependent workflow and *Template* should be deleted. This policy makes critical the problem of changing the Graph structure of a workflow under development.

3.1.2.1.1.1 Modification the graph of an existing workflow

The solution is the following: The graph under an existing workflow can be changed. As a single graph may be connected to several workflows a special, two step measures are enforced in order to avoid unintended update of other workflows:

1. The *Edit* button opens the **Graph editor** where the actual graph can be modified. The user is instructed to use the Save as menu button to associate a new name to the modified graph.
2. The usage of the Fit copied workflow to a new graph button prompts the user to select a graph and create a new workflow with it. It is suggested that the user selects the graph has been created in Step 1. The confirmation of this operation sets the focus of the configuration on the new workflow which inherits its configuration from the original one.

Example: Let us start from the graph G1 containing jobs J1 and J2. After we have built workflow W1 dependent on G1 (G1 ->W1) we recognize that we need a third Job J3. Starting the Graph editor by "*Edit*" we use Graph editor's Save as function to create the clone G2 of G1. As G2 is not bound we can edit it in order to contain J3. In the subsequent step, using the button "*Fit copied workflow to a new graph*" the graph G2 will be selected to create the Workflow W2 and the settings in the environment of J1 and J2 will be preserved. (See Appendix Figure 12.)

3.1.2.1.2 Cloning of an existing Workflow

This operation can be performed by selecting "different Workflow" of the choice "Create a new workflow from a" in the tab Workflow/Create Concrete (See Appendix Figure 5)

The associated opening list box encounters the names of available existing workflows to select from. A new copy of the existing workflow can be created. The Graph reference of the original Workflow will be preserved. The job configuration history of the original workflow is not copied.

3.1.2.1.3 Using a template to create a new Workflow

This operation can be performed by selecting "Template" of the choice "*Create a new workflow from a*" in the tab *Workflow/Create Concrete* (See Appendix: Figure 5).

The associated opening list box encounters the names of available existing templates to select from. The graph defined in the template is preserved. A template defines a set of immutable features; these cannot be altered in an eventual subsequent modification (*Workflow configuration*) process.
Similar to the Graph reference the reference to the template is preserved. Workflows created by a template are sometimes referenced as "*templated*" workflows. Applications used by a common user or workflows which are used as embedded workflows must be "*templated*".

3.1.2.1.4 Uploading of a previously downloaded workflow.

This operation can be selected in the tab *Workflow/Upload*. (See Appendix: Figure 37)
A workflow, which has been stored previously in a local archive (in the client machine of the user) can be uploaded. A workflow must have a graph and may have a template binding; the proper graph (and *Template*) is uploaded together with the workflow.

At present in case of name collisions, which are not permitted, the system does not match the content of the new graph (and template) with the existing ones.

To avoid these collisions the user has the possibility to rename the uploaded workflow and the bound graph (and *Template*) during the upload process. Details of import are discussed in the Appendix describing the *Upload* menu.

3.1.2.1.5 Import of a previously exported workflow

See Appendix: Figure 25 *Import* menu.

This operation can be selected by one of the named items whose type is "*Concrete*" or "*Application*" or "*Project*" in the tab *Workflow/Import* (See Appendix Figure 38). This case is similar to *Upload* but differs from it in several respects:

- The source of Upload is not a local archive, but the so called Repository, which is a common database among all users of the Portal. The Repository is permanently accessible by the portal server. Experienced Users have write permissions to it, i.e. they can *Export* (Publish) their own full workflows (and parts of them) and all users have Import right, they can copy the repository items found there.
- The other difference is that that the repository items are not constrained to *Workflows*, but can be *Graphs*, *Templates*, *Applications* and *Projects* as well.
- As 3.7.1 states the import of an "*Application*" or "*Project*" may involve the import of more than one workflow: If a workflow definition contains references of called (**embedded**) Workflow(s) then the definition(s) of **embedded workflow(s)** must be imported as well.
- Note that this statement is a recursive one, and in the reality the transitive closure of the workflow definitions are uploaded.
- There is an automatic renaming process: During import a unique string is appended to the respective names (of workflow, graph, template) in order to avoid name collisions.

In addition, even the prefix of names can be changed, the same way as it has been discussed in *Upload*. Details of import are discussed in the Appendix describing the Import menu.

3.1.2.2 Workflow Modification

Modification means the configuration of a workflow. This operation can be selected by the button *Configure* in the tab *Workflow/Concrete* in the line of the workflow to be modified. (See Appendix Figure 6) Upon selection this button the user gets the workflow configuration window: See Appendix Figure 12. The modification may happen in three subsequent steps:

1. Eventual replacing the Graph of the workflow with a different one as explained in (3.1.2.1.1.1) in order to change the topology of the workflow.
2. Configuring the jobs in any order, where the jobs are selected by clicking on the proper icon of the displayed graph. Job configuration is detailed in Chapter 2.
3. Saving the configured workflow on the server, by the button "*Save on Server*"

Saving involves the uploading of those input end executable files referenced in workflow description, which are in the local archives of the user. Upon upload the user can decide to delete all instances belonging to the previous configuration of the workflow.

3.1.2.3 Workflow Deletion

This operation deletes the workflow and the eventual workflow instances of it from the list of the given user.

This operation can be selected by the button "Delete" button in the tab Workflow/Concrete in the line of the workflow, which is to be deleted. (See Appendix Figure 6.) The operation needs confirmation.

3.1.2.4 Workflow Publication

This operation exports the definition of given workflow for the user community by placing the definition in the Repository.

This operation can be selected by the button "Export" in the tab Workflow/Concrete in the line of the workflow, which is to be exported. (See Appendix Figure 6)

Upon selection this button the user gets the Export "pop up" form: (See Appendix Figure 42). The selected workflow can be exported in any of the following three selectable roles:

1. Application: The system regards this application "semantically defined". As the workflow may have references to embedded workflows the definition(s) of embedded workflow(s) -and the transitive closure of it (them) – is (are) investigated and exported together with the main Workflow. The export is refused, if the application is not correct. The details of failures can be checked by the button Info in the tab Workflow/Concrete in the line of the workflow, which is to be exported. Note: Info indicates the lack of a proxy certificate, needed for job submission as well. However the goal of the Export is the usability of the given workflow in a later time, eventually by a different user, therefore the existence of a valid proxy certificate is not condition of the export.
2. Project: The Project role slightly differs from the Application. The system does not control the fullness or correctness of the workflow, regarding it "under construction".
3. Workflow: The Workflow role differs slightly from the Project role. The eventual embedded workflow references are not taken in account, i.e. eventual embedded workflows are not exported together with the main workflow.

3.1.2.5 Workflow Abstraction

In order to support reusability, the developer user is entitled to abstract workflows by the creation of - so called - Templates from the existing workflows. With OO terminology Templates are abstract super classes of workflows containing finite elements, not modifiable by the derived workflows. Templates are discussed detailed in Chapter 3.6.

3.1.3 Operations of common user

The common user can only

- import (See 3.1.3.1)
- modify (See 3.1.3.2)
- delete (See 3.1.3.3)
- the given workflow if it is of Application type.

3.1.3.1 Import an Application

See Appendix: Figure 38.This operation can be selected by the value "Application" value in the tab Workflow/Import.

(See the Chapter 3.1.2.1.5 Import of a previously exported workflow, where it must be noted that the common user can select a Repository item only from the list of Applications).

3.1.3.2 Modify an Application

This operation can be selected by selecting the *Configure* button on the tab *Workflow/Applications*. (See Appendix: Figure 41.) A simplified form appears where all definable parameter are listed in a single page.

The form can be posted by the *Save on Server* button. The labels and the optional, icon hidden descriptors identifying and explaining the listed entries which have been created by the Developer User, who - by selecting a Template entry to be "open" - must have defined a proper label and may have added additional comments – the descriptor- in order to instruct the common user. The values of parameters which cannot be modified by the common user are not shown. As the application may include several embedded workflows, the generated configuration list collects all open Template entries gained from all Templates.

Pitfall: It is a well-known problem, that it can occur that the labels coming from different templates are the same, or two workflows within the application have a common Template. The consequence is, that the generated parameters can be indistinguishable for the common user.

3.1.3.3 Delete an Application

See Appendix: Figure 40. This operation can be selected by selecting the *Delete* button on the *Workflow/Applications* tab. This operation deletes the application and the eventual – single - Workflow Instance of the main workflow associated to the application from the namespace of the given user.

3.2 Workflow Submission

3.2.1 Introduction to workflow submission

A workflow can be submitted using three different ways, according to the type of the event triggering the submission:

- Interactively, when the user manually starts the workflow (See 3.2.2)
- In a predefined time (See 3.2.3)
- Responding a web service call of a trusted client machine (See 3.2.4)

Warning: In each case, the user must have a valid proxy certificate for all requested resources. In the interactive case, the user can control the existence of the proxy certificate with invoking the Info command by pressing the button Info in the tab Workflow/Concrete.

3.2.2 Interactive Workflow submission

Both the full power and the common user can submit a workflow, however in lightly different environment.

These user groups can decide to receive e-mail notification about important events of workflow execution.

The e-mail notification can be requested in the *Message* box appearing upon the pressing the Submit command (See Appendix Figure 7).

To confirm the submission command the user can request an optional e-mail notification and can select the class of events in the occurrence of which he/she wants to be notified.

The options are the followings:

- The user never receives notification in the default case.
- The user receives notification, upon termination of the workflow instance
- The user receives notification, about each change of the state of the workflow instance. (States of workflow instances are discussed in chapter 3.3)

The proper filling of the Notification menu (tab New features Setting/Notify) is the precondition to receive an e-mail. This form has two logically separated levels: The address part must be defined in the pan "e-mail general settings", in the pans "Message about change of Workflow state" and "Message about trespassing of the threshold of Storage quota" pans the user has to define the content part of the message to be generated. Both the address part and the content parts should be enabled for the proper message generation.

Messages can be generated even in loosely related cases to the submission of an individual workflow: A user may be notified if the quota of *Storage* is exhausted. (The quota is allocated by the System Administrator to maintain the user data on the portal Server. See more detailed in 3.7)

3.2.2.1 Workflow submission by a full power user

Experienced users may start their workflows, selecting one from the list encountered in the tab *Workflow/Concrete* tab by the button Submit. (See Appendix: Figure 6.) Chapter 3.1.2.1 describes the way how a workflow can be added to the list. Upon submission a new instance of the workflow is created.

To identify the instances a user defined, "optional notes on instance" can be assigned to the instance, in the same *Message* box, where the submission must be confirmed, and the e-mail notification is requested. (See Appendix Figure 7)

The default value of this note is the date and time of the submission. All instances of a given workflow with their notes are listed (and accessible for view or manipulation) by pressing the button *Details* in the line of the workflow, in the *Workflow/ Concrete* tab. See Appendix Figure 8 and the Chapter 3.4

3.2.2.2 Workflow submission by a common user

See Appendix: Figure 40. Common users can start their workflow applications, selecting one from the list encountered in the *Workflow/Applications* tab by pressing the proper *Submit* button. Chapter 3.1.3.1 describes the way how an application can be added to the list.

Note that – other as in the case of the developer users - there is only just a single instance, upon a successful workflow submission. The eventual former one is deleted upon submission.

3.3 Workflow States and Instances

The state of a workflow instance can be any of the followings:

- **Submitted**
- **Running**
- **Finished**
- **Error**
- **Suspended**

The initial state "*Submitted*" is associated to a new Workflow Instance created by the command submit executed on a workflow.

The state of the workflow instance is "*Running*" if the first component job instance reaches the job state "running".

Jobs have their own run time states and therefore instances as well. In case of PS workflows (See 2.6.3.1.2) a job can be submitted several times within the same workflow instance due to the set of file contents associated with one or more input port(s). It means that jobs can have several instances within the same PS Workflow instance. The state of the workflow instance is "*Finished*", if the workflow has executed each of the intended job sequences, and has not executed the intended omissions.

The intended omissions are defined by the followings: A subsequent job must not be executed in any of the two special cases:

1. Either a user defined condition on an input port is false (job state is "*term_is_false*") or
2. the actual number of output files in a Generator is exhausted (job state is "*no_input*").

Certainly, the intended omission does not cover the situation, if a job does not receive an input file due to a network error or due to an abortion of any kind of a preceding job. Important notice:
However for the time being the current implementation does not separates the *no_input* (1) job state due to the intended omission from the *no_input* (2) job state due to configuration or run time error. The result is, that in some cases a "*Finished*" state of a workflow instance may hide erroneously configured jobs. The workflow instance is doomed to be in the final state "*Error*", if any of its jobs remain in the "error" state. However, even in this state the system tries to submit each job, which has the needed data on its input ports. If a workflow has not reached its "Finished" state, then it can be suspended by a user's interrupt.
Suspending means that the execution of all jobs, which are running will be aborted, and the aborted jobs become in *init* state.

The execution of workflow, which is in "*Suspended*" or on "*Error*" state, can be resumed by the user's intervention. Resume means that the jobs, which were in "error" state become in init state, and interpretation of workflow instance is continued for all job instances, which are in "*init*" state and can be submitted. A workflow instance in static states ("*Suspended*", "*Finished*", "*Error*") can be deleted as well. The suspension of the execution is propagated in the embedded workflow instances: these are aborted. The resume operation starts new instance of the embedded workflows.

3.4 Observation and Manipulation of Workflow Progress

Common and experienced users have different methods to verify and control how a workflow execution evolves and terminates.

3.4.1 Methods of a common user

The *Workflow/Applications* tab serves the common user to start, observe and stop a workflow. (See Appendix Figure 40) As a basic assumption, it is asserted that a common user deals only with tested workflows.
First of all the common user is interested in the observation of reaching the end states.
The *State* information (see 3.3) gives comprehending information about the state of the workflow and the user can receive "offline" notification about the progress of the workflow, using the e-mail notification mechanism (See 3.2.2).
Moreover the common user may be interested in suspending a running workflow.
It may occur if

- the user is not interested in the result any more (the execution time of the program exceeds the user's expectation an it is assumed, that there is an underlining middleware, network or resource error); or
- the user has detected his/her own setting error and wants to repeat the experiment.

The suspending of the workflow can happen by pressing the *Suspend All* button. This button is visible only if the corresponding application is running.
The state of the suspended workflow is *Suspended*. The suspended workflow can be resumed by the *Resume* button or reconfigured and subsequently saved by pressing the *Configure* button (see 3.1.3.2). The reconfiguration deletes the workflow instance. Finally, by pressing the *Delete* button the workflow instance and the workflow as well will be deleted.

3.4.2 Methods of a full power user

The developer user has online and off line methods to observe the running instances of a workflow. The off line method is the e-mail notification discussed in Chapter 3.2.2.

As the workflow execution spreads over the grid, it evolves the following way: workflow -> workflow instance -> job -> job instance. The levels of observation and the interaction follow these four levels of abstraction as well.

3.4.2.1 Highest level: Workflow

The *Workflows/Concrete* tab displays a statistical summary about the number of workflow instances of the given workflow, which can be in any of the main states: **Submitted, Running, Finished, Error**. The statistical summary does not display the workflow instances which are in Suspended state. See Appendix Figure 6.If there isn't any workflow instance, which has been submitted, but not terminated (i.e. the sum of Submitted + Running is = 0), then the button Delete becomes visible in the line belonging to the given workflow, and the whole workflow together with it's all eventual instances can be deleted. In the altering case, another button, "*Suspend all*" appears in the proper line. Using this button, each submitted workflow will be suspended. Pressing the button Details, the next lower level of manipulation and visualization is opened in a new page, listing the individual workflow instances, belonging to the selected workflow: See below: 3.4.2.2

3.4.2.2 Workflow instance list level

The workflow instance list level displays the existing instances of a given workflow. See Appendix Figure 8.The workflow instance states and buttons of manipulation functionality (*Details, Suspend/Resume, Delete*) belonging to the individual workflow instances are listed on this level.
The "missing" workflow instances being in "*Suspended*" state not referenced on the highest level are encountered here as well. Similar to 3.4.2.1, the *Delete* and *Suspend* buttons appear alternatively, depending from the termination state of the workflow instance.

The *Suspend* operation means the killing of job instances, which are in running or in submitted state and reset them together with job instances being in error state in *init* sate. Shortly speaking, the suspend operation executes a job instance level check pointing, saving only those job items, which terminated properly (being in state finished) and sets back the system to be ready to continue its working, using the outputs of the properly terminated job instances. The state of the workflow instance will be *Suspended* and the calculation can be continued by pressing the appearing *Resume* button, or the whole workflow instance can be erased by pressing the other button appearing in this state, the *Delete* button.

Pressing the *Details* button extends the page by opening a one level deeper structure of the workflow: It is an overview of job instances, belonging to the selected workflow instance. See below 3.4.2.3

3.4.2.3 Overview of job instances level

See Appendix Figure 9. On this level the view of the selected workflow instance is extended by the jobs and job instances. The instances of a given job type, are further subdivided, according to their current state, i.e. there is a separate line for each set of instances of a given job, being in the same state. The number of the elements of the given set is also displayed in the column Instances. So, the displayed table has three display columns:

1. Job, for job names occurring in the workflow
2. Status, for the job instances being in that job state
3. Instances, for the number of elements in the set.

Note, that the table is dynamic, e.g. those jobs, which have not been touched yet, during the interpretation of the workflow instance in the moment of visualization are not displayed. It means, that the number in the column "Instances" may not be 0 and if its value is greater than 1 it is a clue of the parametric nature of the workflow. Pressing the button "View Content(s)" extends the page by the individual encountering of job instances. See below 3.4.2.4.

3.4.2.4 Individual job instance level

On this level the view of the selected workflow instance is extended by the instances of a selected job being in a given state.
There may be a big number of instances for a single job therefore a new paging method has been introduced since the release 3.2: Only a fraction of the instances will be displayed in ascending PID order on the page if the number of jobs being the given state(s) exceeds the limit indicated in Range. The initial element of the actual range can be set by *From*. (See Appendix Figure 10.)

The meaning of *From* can be altered by selecting the actual argument (Method 1 or Method 2) of Sorting Method.

However the two methods give different results only in the intermediate workflow state, where not all job instances are in their final states:

- **Method 1**: From serves just paging in the result set i.e. the PID index of the first displayed job instance may be less than the value of *From*.
- **Method 2**: From is used to select the first job instance of interest whose PID is not less than the value of From, and only the instances are shown whose PID-s are less than the sum of values of From and Range (From <= PID < FROM+ RANGE)

The sorting operations are validated by the *Refresh* button. There is separate line for each job instance. As job instances are the traces of job execution activities, the produced output files can be accessed using the associated buttons:

- Logbook displays all log information collected from the various levels of job submission system. These are generally java and script printouts commenting the execution of the job.
- *std.Output* displays the "stdout" file content, when the task enveloped in the current job instance has written in the standard output file. (See Appendix Figure 11)
- *std.Error* displays the "stderr" file content, when the task enveloped in current job instance has written in the standard error file.
- Download file output opens the browser dependent download mechanism by which a special compressed file will be downloaded from the server to the machine of the client.
- This file contains all local (not remote grid) output files, which have been produced by job instance on its standard outputs (stdout, stderr) and on the output(s) having been mentioned in the port specification(s) of the corresponding job.

3.5 Fetching the Results of the Workflow Submission

Workflow elaboration may produce local and remote output files.

3.5.1 Remote grid files

Remote output files are stored in **Storage Elements** and – from the portal's point of view -, those files don't belong to the individual workflows any more. As the names of them is well known by the user, they can be accessed by a separate service of the portal, namely by the *File Management* menu.

3.5.2 Local files

The common and the developer user have different methods:

3.5.2.1 Access to local output files by the common user

In the *Workflow/Application* tab the availability of the result is indicated by the existence of the button *getOutputs*. See Appendix Figure 40 where this button does not appear.

3.5.2.2 Access to local output files by the full power user

Local output files can be accessed and downloaded

- either in "little" packages, associated to a certain job instance (See 3.4.2.4) or
- by using the tab Workflow/Storage.

The *Storage* menu gives –among others – a wide range of possibilities to download the result of

- a single selected workflow instance, i.e. the collection of all job instances belonging to it
- all instances belonging to a given workflow. (See more detailed in 3.7)

3.6 Templates for the Reusability of Workflows.

3.6.1 Introduction to Templates

Templates have been introduced to support the reusability of defined and tested workflows. To be more specific three goals are envisaged:

1. Simplified redefinition of a workflow;
2. Type checking of the "plug in" ability of an embedded workflow, where the embedding is made more secure by requiring that an embedded workflow must be "templated" one, which means that the embedded workflow must have been defined with the help of a template;
3. Assistance in creating the simplified user interface for the common user automatically, on the base of template description.

What is a template? A template is an extension of a workflow definition, in such a way, that each configurable job or port related atomic information item is extended – at least - by an immutable Boolean value. The values of these Boolean metadata are mentioned as "*Free*" and "Close", respectively. "*Close*" means, that the related atomic configuration information item is immutable, i.e. in each workflow, which references a given template the closed atomic configuration information item is preserved, it cannot be changed, during the workflow (job) configuration process. "Free" means that the value of the related atomic configuration item is copied as default, but it can be changed by the user. Related to the "*Free*" state of the Boolean value, two other metadata can (and should) be defined:

1. The first is a short string *Label* identifying the given piece of information, which can be changed, and
2. the optional description may give a detailed description of the usage, either syntactically or semantically. Please note, that the workflow configuration form used by a common user (See 3.1.3.2) is generated upon these metadata.

3.6.2 Life cycle of a template

A template is a named object and it must be created based on a workflow. (See 3.6.2.1)
Subsequently, the created Template can be used to serve as a base of creating the definitions of new workflows. (See 3.1.2.1.3) It follows from the way of creation the Templates that the referenced Graph of the base workflow inherited in the Template and subsequently, in the workflows, which have been created upon Templates. Workflows mentioned above have beside the Graph name reference a

Template name reference as well. These workflows are called "*Templated*" workflows. The use of "*Templated*" Workflows is obligatory in the following positions:

- Workflows used to be embedded in other workflows. (See 2.1.3)
- Workflows exported as Applications (See 3.7.3)
- Workflows used to create Template by derivation (See 3.6.2.1.1.2)

3.6.2.1 Creating a new Template

Templates are created in the tab Workflow/Template, which lists all existing Templates of the user. Because of historical causes, Workflows and Templates have a common namespace (See Appendix Figure 32.)

During the creation (more precisely - during the including configuration) of a template each atomic information item will be defined and there is no possibility to modify the metadata defined by the Template afterwards, i.e. at present the Template is an immutable object. The creation of the template can be subdivided in two sub processes:

1. Creating a new named Template object, associated with an existing reference workflow (See 3.6.2.1.1)
2. Configuring the template, deciding about the *Close/Free* status of each configurable feature of the reference workflow. (See 3.6.2.1.2)

3.6.2.1.1 Naming the new Template and select a reference Workflow

By choosing a reference workflow we have two options:

1. Use a general workflow (See 3.6.2.1.1.1);
2. Inherit the restrictions of a chosen "Templated" Workflow. (See 3.6.2.1.1.2)

3.6.2.1.1.1 Use a general workflow as reference

This option is selected by the choice "*Select a concrete workflow as base to create a template*"
In the corresponding list box all workflows of the user are enumerated. The selected workflow can be "*Templated*" as well. In this case the metadata (the Boolean values, Labels and Descriptions) can be used as defaults, which can be overruled during the subsequent Template configuration process.

3.6.2.1.1.2 Derivate a "Templated" Workflow

This option is selected by the choice "Select a templated concrete workflow as base to derive a template". The corresponding list box numerates only such workflows of the user which have been created by a template i.e. which are *Templated Workflows*.
In this case the user may decide during the subsequent template configuration process only about the closing of the free configuration information items of the reference workflow, i.e. the closed configuration information items of the referenced workflow remain closed.

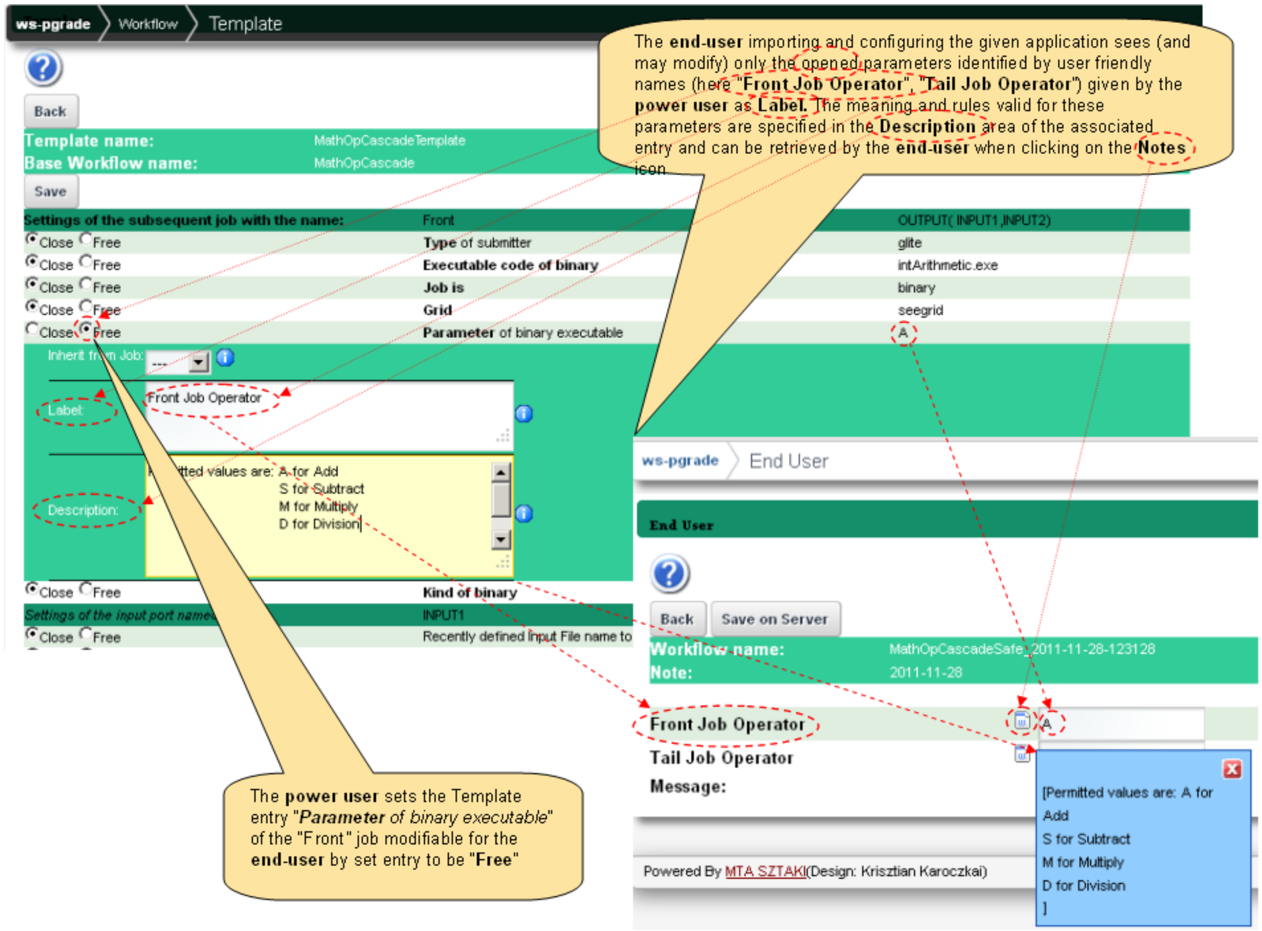
3.6.2.1.2 Configuring the Template.

The button Configure on the *Workflow/Template* tab opens a new listing form. It is a rather long list, where each configured workflow features can be decided upon. The features can be identified by the same or similar string identifiers as they referenced in the windows describing the job- and port property configuration (see Chapter 2). See Appendix Figure 33 for the configuration list. The listing of the features – called atomic information items - is grouped by jobs following the workflow/job configuration hierarchy.
The items contain tree elements:

1. The Boolean metadata whose value can be selected by a Close or Free choice of the radio button;
2. the name of the atomic information item;
3. the value of the configuration item which can be frozen by selecting the option "Close"

Note that the items are grouped and introduced by a header line "*Settings of the subsequent job with the name:*" < name of job >

For the time being, the modifiable default values of the Boolean metadata are set as "Close".
If the user selects Free, the associated label and description become editable. The value defined as Label will appear as label in the simplified application dependent configuration form of the common user.
The value defined as Description can be read by the common user clicking on the proper "Notice" icon in the simplified application dependent configuration form. To accelerate the configuration the following help option can be used:
If a proper existing label - description pair has been defined for a foreign job, the same pair can be copied here by referencing the list box "*Inherit from Job*:". The configuration must be confirmed by the *Save* button. The next figure explains the effect of the configuration. The left side of the figure is a detail of Appendix Figure 33 and the right side of the figure is a detail of Appendix Figure 41 showing such an application whose workflow has been created with the help of the shown template (Figure 10.)



Template name: MathOpCascadeTemplate
Base Workflow name: MathOpCascade

Settings of the subsequent job with the name:	Front	OUTPUT(INPUT1,INPUT2)
● Close ○ Free	Type of submitter	glite
● Close ○ Free	Executable code of binary	intArithmetic.exe
● Close ○ Free	Job is	binary
● Close ○ Free	Grid	seegrid
○ Close ● Free	Parameter of binary executable	A
● Close ○ Free	Kind of binary	
Settings of the input port name	INPUT1	
● Close ○ Free	Recently defined Input File name to	

Inherit from Job: ---

Label: Front Job Operator

Description: itted values are: A for Add
S for Subtract
M for Multiply
D for Division

Workflow name: MathOpCascadeSafe_2011-11-28-123128
Note: 2011-11-28

Front Job Operator: A
Tail Job Operator
Message:

[Permitted values are: A for Add
S for Subtract
M for Multiply
D for Division
]

Powered By MTA SZTAKI(Design: Krisztian Karoczkai)

The **end-user** importing and configuring the given application sees (and may modify) only the opened parameters identified by user friendly names (here "**Front Job Operator**", "**Tail Job Operator**") given by the **power user** as **Label.** The meaning and rules valid for these parameters are specified in the **Description** area of the associated entry and can be retrieved by the **end-user** when clicking on the **Notes** icon

The **power user** sets the Template entry "*Parameter of binary executable*" of the "Front" job modifiable for the **end-user** by set entry to be "**Free**"

Figure 10 Consequence of the configuration of a template on the simplified configuration interface of the related Application

3.7 Maintaining Workflows and Related Objects (Up-, Download and Repository)

3.7.1 Introduction

Originally, the workflows are created and stored on the Portal Server (See 3.1.2.1)
The created workflows and related objects (graphs, templates), and the results of workflow submissions can be archived (downloaded) to the desktop machine of the client. Beyond the trivial case that the user wants to fetch the result of workflow submission the download may be necessary, if the user wants a security copy, needs to migrate to another portal, or must delete some objects because he/she has exhausted his/her storage quota on the portal. This operation can be done in the proper listing tab of the given object (*Workflow/Storage, Workflow/Graph, Workflow/Template*) by selecting the button Download belonging to the line of the selected item. The objects can be subsequently uploaded using the methods defined in *Workflow/Upload* tab.

Note: a user can upload an object even when, it has been created by a different user. The more advanced form of the applications publication is the Export – Import mechanism:

A full power user can make a created object (Graph, workflow, Template) public by exporting it together with an optional description in a database called **repository**, which is accessible by all users of the WS-PGRADE portal. The most important objective of the repository is the publication of applications.

An application is a tested workflow with defined semantics, where generally at most the input files, the command line parameters and the resources of jobs can be altered by the end user. As an application may contain calls of embedded workflows, the definition of referenced embedded workflows are included in the definition (and in the representing file package) of the application as well. As the applications may be imported and used by common users as well, and the common user can configure only a "*Templated*" workflow, it is required that the workflows involved in an application must be created with Templates. A Project is another kind of workflow collection, which can be exported. Other than in the case of an Application, it is not required that the selected workflow be tested and semantically complete. Rather it is an "under construction" application, which has to be saved with all the referenced objects. After this introduction; it becomes clear that a selected concrete workflow can be exported – in a given case - by three different ways:

- as an *Application*: tested to be semantically complete, being template and packed together with all referenced objects.
- as a *Project*: no testing and packed together with all referenced objects
- as a *Workflow*: no testing and prepared to copy not including the eventually referenced embedded workflows.

3.7.2 Download detailed

Technically, the downloading means the collecting and compressing of the needed files on the WS-PGRADE Portal server and letting the download facility of the used web browser to control the physical file transfer to the client machine.

The downloading of a workflow involves in all cases the downloading of the referenced *Graph* and - if there is a referenced Template (defined by the workflow) - then the downloading involves the definition of the *Template* as well.

3.7.2.1 Download by a common user

The common user can only download the results of the submitted workflows (See 3.5.2.1).

3.7.2.2 Download by a full power user

Graphs and *Templates* can be downloaded independently pressing the button Download button in the *Workflow/Graph* tabs (see Appendix Figure 1) and *Workflow/Template* (see Appendix Figure 32) respectively. The advanced (developer) user has the *Workflow/Storage* tab (see Appendix Figure 36) to download the objects related to a given workflow to the client machine.

This tab enumerates not only the workflows, but the instances created from the given workflows as well:

3.7.2.2.1 Download of Workflow Instances

In the line belonging to the given workflow, the column Instances enumerates the list of instances to be select from. As the instances of a given workflow may differ, there is a possibility to download the compressed collection of the local output files, which were produced separately by a selected workflow instance. (See the button *get Outputs*).

Not only the outputs but the whole workflow instance – containing the workflow definition can be downloaded by the button "*get Instance*"

Warnings:

Please note, that up to now – and against justified user expectation – the downloaded content of the workflow instance will not reflect the contemporary configuration of the workflow but rather the last modification of the workflow:

Let us suppose that the workflow named "W" –including Input_1 has produced the instance W-instance_1 including Output_1.

Replacing the input of the workflow to Input_2 and submitting the W again the same workflow will produce the W-instance_2 containing Output_2. If the user downloads the former instance - W-instance_1 - it will contain the later input Input_2 instead of Input_1.

3.7.2.2.2 Download of Workflows

The buttons of the column group Download Actions refer to not only an individual workflow instance, but to the whole workflow:

- "*get All*" downloads the workflow with all instances (including the local outputs of all instances).
- "*get All but Logs*" downloads the workflow definition and the local files produced on the ports of the workflow, without the log files.
- "*get Inputs*" downloads the recent local files, which have been uploaded to the input ports of the workflow.
- "*get Outputs*" has the same effect as the get Outputs command (discussed in 3.7.2.2.1) - but issued for each instance.

3.7.3 Export to the Repository

Export is a group of operations (reachable in *Workflow/Graph, Workflow/Concrete, Workflow/Template* tabs) which make objects reusable for other users of the portal.

Export can be regarded as a high level "download", using the same compression method to archive the requested objects. However, it results an entry in the Repository. As mentioned, in the introduction (see 3.7.1) in case of the export of a workflow (*Workflow/Concrete* tab) a classification must be done, how the workflow is exported. (See Appendix Figure 42)In case of a qualification "*Application*", an additional test about the correctness and "*Templated*" kind of the workflow is performed.

3.7.4 Upload

Upload means the reloading of an object in the WS-PGRADE Portal Server from a local file archive of the user, where the entry in the local file archive must be the result of a previous *Download* operation.
The Upload operation can only be performed by a full power user using the *Workflow/Upload* tab (See Appendix Figure 37)

1. The source of the upload is a properly compressed file in the directory of the client selected by the file browser. Upload is the inverse process of download. Named downloaded objects (graphs, templates, workflows and workflow instances) can be put back in the storage, allocated for the user on the portal server. As the objects can appear with their original names among the other objects, name collision might occur which is not permitted.
2. To avoid name collisions the user can rename the object on the fly, during the upload process. As the upload of a workflow involves the upload of a graph and may involve the upload of a Template (See 3.7.2), there are three input fields for the eventual redefinition of names of the requested object types. The renaming requests must be marked on the associated check boxes.
3. The upload operation must be confirmed by the button Upload.

3.7.5 Import from the Repository

See Appendix Figure 25. The Import operation – the inverse operation of Export - can be executed by any type of users. Import means the copying of a Repository object in the proper reusable object library (libraries) of the user.
It must be done on *the Workflow/Import* tab (see Appendix Figure 38). This tab shows the list of importable objects (with the eventual associated comments) belonging to the selected segment of the Repository.
The selection corresponds to the roles given upon *Export*:

- Graphs exported from the *Workflow/Graph* tab
- Templates exported from the *Workflow/Template* tab
- Workflow exported as workflow from the *Workflow/Concrete* tab
- Project exported as Project from the *Workflow/Concrete* tab
- Application exported as Application from the *Workflow/Concrete* tab

Note: To avoid the name collision problem mentioned at Upload (see 3.7.4) the names of imported objects are systematically renamed by postfix string coding, which is a unique number. Please remember the import (in case of Project and Application) may involve the indirect import of the referenced embedded workflows objects. The "postfixing" of names is extended to their names as well. Moreover, the user has the possibility to change prefix of the names of the imported object the similar to that way has been discussed in case of upload (see 3.7.4).

However, the prefix renaming has no effect on the objects belonging to the embedded elements. The import can be executed in the following steps:

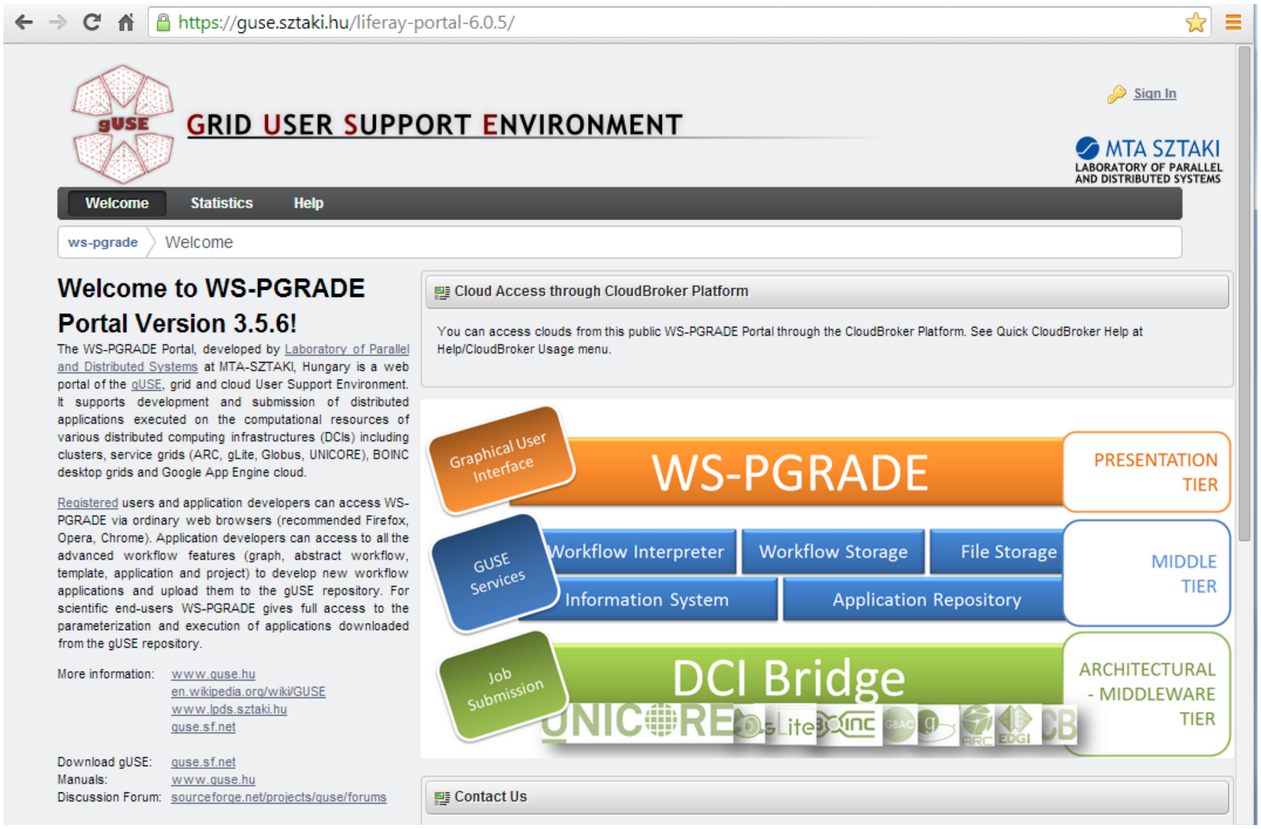
1. Select the type of the repository objects by list box "Select type"
2. Show the selected items pressing the button "Refresh /Show List"

3. Select the object to be imported by setting the proper token of the left side radio button
4. (Optional step) rename the prefix of the object name using the fields "renaming options"
5. Select the proper operation (beside the default Import the full power user has the right to delete the selected object, selecting the action type as Delete)
6. Confirm the command using the button Execute.

4. Access to the gUSE Environment

This chapter summarizes organization of the portlet structure of the WS-PGRADE Portal in order to access the gUSE infrastructure. The individual portlets are described detailed in proper chapters of Appendix I.

4.1 Sign in the WS-PGRADE Portal


https://guse.sztaki.hu/liferay-portal-6.0.5/
gUSE
GRID USER SUPPORT ENVIRONMENT
Sign In
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Statistics
Help
ws-pgrade
Welcome
Cloud Access through CloudBroker Platform
Graphical User Interface
WS-PGRADE
PRESENTATION TIER
GUSE Services
Workflow Interpreter
Workflow Storage
File Storage
Information System
Application Repository
MIDDLE TIER
Job Submission
DCI Bridge
UNICORE
gLite
BOINC
GBAC
ARC
EDGI
CB
ARCHITECTURAL - MIDDLEWARE TIER
Contact Us

Welcome to WS-PGRADE Portal Version 3.5.6!

The WS-PGRADE Portal, developed by Laboratory of Parallel and Distributed Systems at MTA-SZTAKI, Hungary is a web portal of the gUSE, grid and cloud User Support Environment. It supports development and submission of distributed applications executed on the computational resources of various distributed computing infrastructures (DCIs) including clusters, service grids (ARC, gLite, Globus, UNICORE), BOINC desktop grids and Google App Engine cloud.

Registered users and application developers can access WS-PGRADE via ordinary web browsers (recommended Firefox, Opera, Chrome). Application developers can access to all the advanced workflow features (graph, abstract workflow, template, application and project) to develop new workflow applications and upload them to the gUSE repository. For scientific end-users WS-PGRADE gives full access to the parameterization and execution of applications downloaded from the gUSE repository.

More information: www.guse.hu
en.wikipedia.org/wiki/GUSE
www.lpds.sztaki.hu
guse.sf.net

Download gUSE: guse.sf.net
Manuals: www.guse.hu
Discussion Forum: sourceforge.net/projects/guse/forums

You can access clouds from this public WS-PGRADE Portal through the CloudBroker Platform. See Quick CloudBroker Help at Help/CloudBroker Usage menu.

Figure 4.1 Welcome Page of the gUSE/WS-PGRADE

New user must follow the *How to get access link* on the www.guse.hu page, on left margin, existing user can log in clicking on the *Sign In* link on the top right corner of WS-PGRADE *Welcome* page (https://guse.sztaki.hu) See Figure 4.1.

4.2 Overview of the Portlet Structure of the WS-PGRADE Portal

Depending on the associated role (the predefined roles are Administrator, Full Power user, End user) the user gets different access to the gUSE whose menu may appear in slightly different forms:

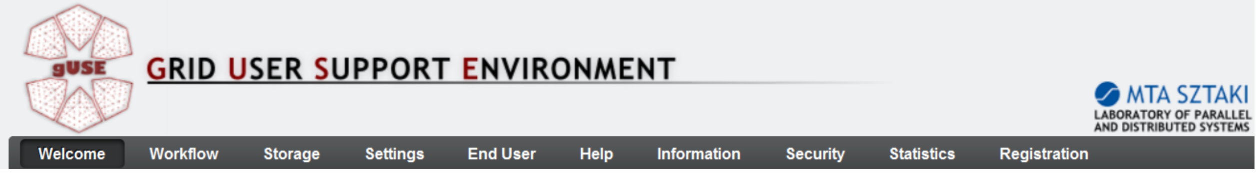

gUSE
GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Workflow
Storage
Settings
End User
Help
Information
Security
Statistics
Registration

Figure 4.2 The main menubar of the gUSE

This chapter summarizes organization of the WS-PGRADE Portal structure.

The elements of the *Workflow* group (*Graph, Create Concrete, Concrete, Template, Import, Upload*) deal with the creation, manipulation and life cycle of workflow related objects.

The elements of the *Storage* group (*Local, LFC*) deal with the
- saving of workflow related objects on the local machine of the user (Local)
- handling of remote grid files (LFC) having been defined in the gLite infrastructure.

The elements of the *Security* group (*Certificate, Public key Assertion*) give support to fulfill the different authentication and authorization requirements stated by the computational resources.

Let be noted that the *Public* key menu registers the respective resources as well. However the resources which require certificate based authentication are maintained in the menu Information/Resources.

The group *Settings* includes miscellaneous administrative activities:
- Notification is accessible for any Full Power and End user. The details of electronic letters to be sent by the system to the user upon workflow related events can be set here.
- Internal Services are accessible only by the Administrator of gUSE. The Administrator can dynamically observe and tune the cooperation of internal components composing the gUSE infrastructure.
- Quota Management is accessible only by the Administrator. The static storage quota from the common and valuable common storage resource of the gUSE allotted to a given user can be set here.
- Text editor is accessible only by the Administrator. Texts and messages of the WS-PGRADE portal are maintained here.

The group Information hides rather different features:
- **WFI monitor** is an experimental development tool to observe the progress of job elaboration within the Workflow Interpreter - which is one of the central services of the gUSE.
- **SHIWA Explorer** is a dedicated browser to explore the remote services using SHIWA technology.
- The new Resources portlet appears only in view (read only) form for the common user and it informs the user about the accessed resources having been added to the DCI Bridge by the System Administrator. The tabs of the portlet represent different (traditional and upcoming) computational technologies and the accessible resources falling in the given category are listed here.

The menu point End User opens directly the End user menu where the end user can import, configure and execute prepared applications.

5. Internal Organization of the gUSE Infrastructure – Only for System Administrators

The gUSE infrastructure connects the WS-PGRADE portal with the remote resources.

In order to support load balancing, scalability, and modularity the gUSE is not a monolithic program but a net of subdivided set of components which communicate with each other by standard service calls. The system administrator has the possibility to change the setup of host machines executing the services dynamically.

To support and understand this maintenance activity the following terms has been introduced:

- A Component Type -sometimes abbreviated as CT - is a named entity, which identifies an insulated activity group. This group is bound by a monolithic code and may have several interfaces which will be referenced in Service definitions. (To the proper work of the gUSE a predefined set of Component Types must be present)
- The configuration of Component Types is detailed in Appendix 17.1
- A Component is a piece of hardware executing the code identified by the Component Type.
- The configuration of Components is detailed in Appendix 17.2

Components may have many parameters which fall in two categories:

1. Obligatory (or generic) parameters (see Appendix 17.2.1)
2. Individual – Component Type dependent – parameters in form of key - value pairs (see Appendix 17.2.2)

The most important obligatory parameters are:

- Component Type: see above.
- Service Group: describes the kind of protocol by which components exchange messages. At present there is just one installed protocol. Its name is "gUSE".
- URL: defines a hardware related access point where internal clients of the Component’s services (clients belong to the gUSE infrastructure) may address their requests.
- URL_to_initialize Component: is a distinguished URL to reset the Component
- Public URL: defines a hardware related access point where external (remote) clients of the Component’s services may address their requests.
- State: Boolean variable (Inactive/Active)

There must be at least one Component to each base Component Type of the gUSE.
It means that the needed activities must be associated to resources by which they can be performed. A Service -which must belong to a given Service Group (see Appendix 17.3) - defines the possible request types among the Components. It has four parameters:

- CT of Server: It is the type of the component which serves the request of the client component.
- CT of Client: It is the type of the client component which requests the service.
- Server side service interface: It is a relative address to find the proper interface elaborating the request on the actual Component.
- Client side interface *impl.class*: points to the definition of the Java class/jar code, which communicates with server on behalf of the client.

It is clear from the definition of the "Service" that if a new functionality - for example a new kind of submitter - is needed then two basic activities must be done:

- Server side: Insert the proper service code and define new service interface to it.
- Client side: Write the implementation of the server-oriented communication using a standardized interface, and declare the access point of this code in the Service entry.

The configuration of an individual Service is detailed in Appendix 14.3.1. The focus of the possible activity of a System Administrator is the set of Components:

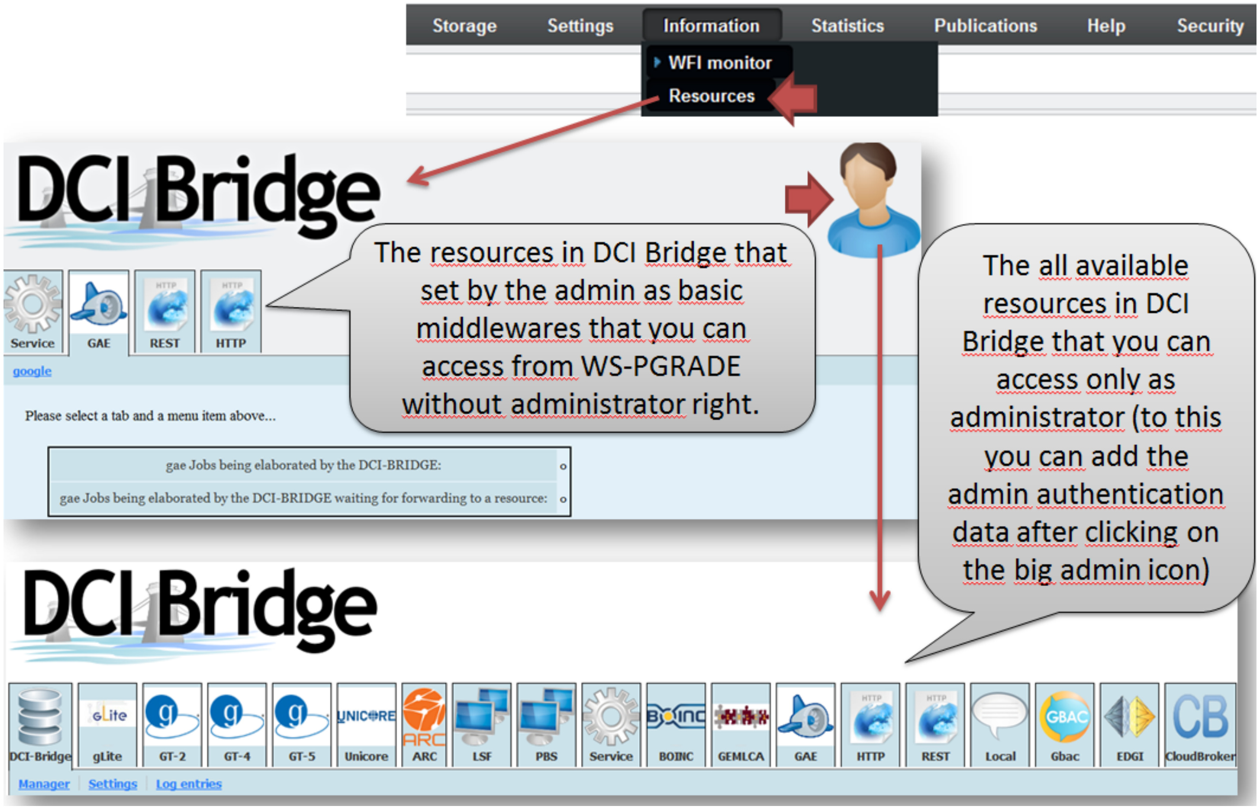
- In case of a malfunction a given Component can be reinitialized by the associated "Refresh" command,
- The services of a given Component can be redirected to different host machine by changing the proper URL parameter
- A secondary Component with the same Component Type can be added to increase capacity/ help load balancing.
- Most probably in this case some Component Type dependent specific parameter must be changed; (this will determine which server Component will serve a given request arriving from a client Component)
- The Component of type submitter has a distinguished role because the back end of the system (the set of access points of the - mostly remote - computational resources) is defined here. The special setting relating the submitter is frequently referenced in the next chapter Resource manager.

6. Resources

6.1 Introduction

The gUSE has a pluggable back end construction by which the resources of different technologies can be connected. The former backend of the gUSE has been replaced by a new uniform service, the DCI Bridge. It replaces the former "Submitters" and serves as a single unified job submission interface toward the (mostly remote) resources (DCI-s) where the job instances having been created in the gUSE will be executed. Together with the introduction of the DCI Bridge the inserting of resources supported by uprising new technologies (clouds and other services) will be simpler and better manageable. The administration of DCI Bridge (adding a new middleware or a new resource to the given middleware, further observing or trimming the flux of jobs toward a given resource) is out of scope of this manual. See the DCI Bridge Administration manual for details. However, the DCI Bridge is available in view form for the Portal user. The Information/Resources menu groups the registered resources according the underlying technology (middleware type). The related resource types are visible on the Information/Resources menu.

You can reach the *Resources* menu by clicking on Information/Resources menu. The appearing window provides to end-users six resource settings possibility (Local, gLite, BOINC, GT-4, GT-5, Service, CloudBroker). Additionally, here you can find information about rough numbers of jobs that are waiting in queues (see Figure 6.1). (Note: this statistics is not available for all resources.) The *Resources* menu itself is accessible by clicking on human head icon on the upper right side. In the appearing dialog box you can enter your authentication data. If it is valid, you reach the Resources menu (see Figure 6.2).


Storage
Settings
Information
Statistics
Publications
Help
Security
WFI monitor
Resources
DCI Bridge
Service
GAE
REST
HTTP
google
DCI Bridge
DCI-Bridge
gLite
GT-2
GT-4
GT-5
Unicore
ARC
LSF
PBS
Service
BOINC
GEMLCA
GAE
HTTP
REST
Local
Gbac
EDGI
CloudBroker
Manager
Settings
Log entries

Please select a tab and a menu item above...

gae Jobs being elaborated by the DCI-BRIDGE: 0

gae Jobs being elaborated by the DCI-BRIDGE waiting for forwarding to a resource: 0

The resources in DCI Bridge that set by the admin as basic middlewares that you can access from WS-PGRADE without administrator right.

The all available resources in DCI Bridge that you can access only as administrator (to this you can add the admin authentication data after clicking on the big admin icon)

Figure 6.1 The way to access Resources menu from WS-PGRADE main menu bar

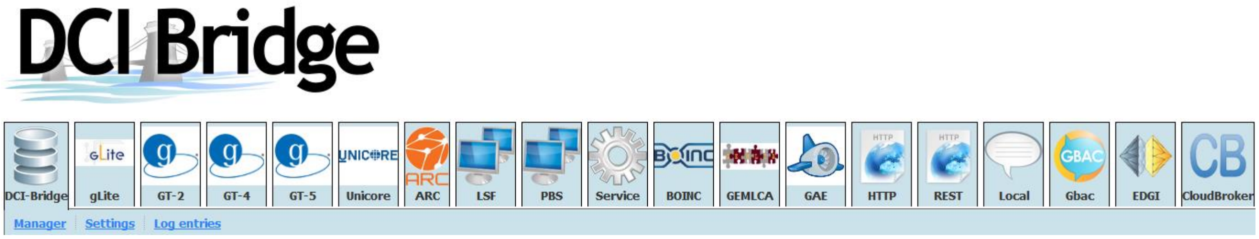
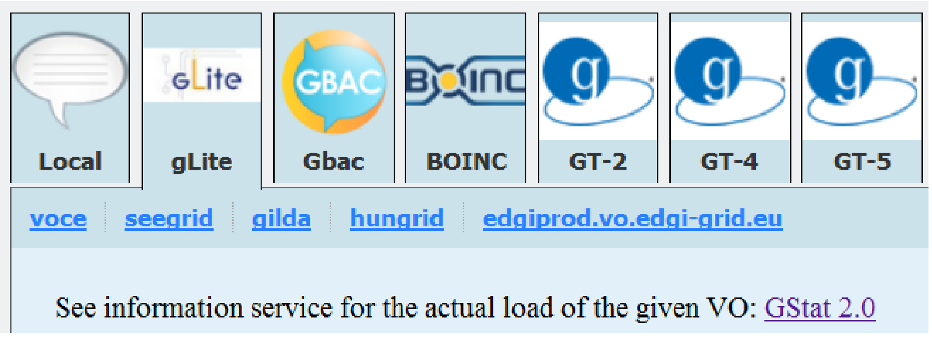

DCI Bridge
DCI-Bridge
gLite
GT-2
GT-4
GT-5
Unicore
ARC
LSF
PBS
Service
BOINC
GEMLCA
GAE
HTTP
REST
Local
Gbac
EDGI
CloudBroker
Manager
Settings
Log entries

Figure 6.2 Resources menu header

6.2 Resources[1]

6.2.1 gLite


Local
gLite
Gbac
BOINC
GT-2
GT-4
GT-5
voce
seegrid
gilda
hungrid
edgiprod.vo.edgi-grid.eu

See information service for the actual load of the given VO: GStat 2.0

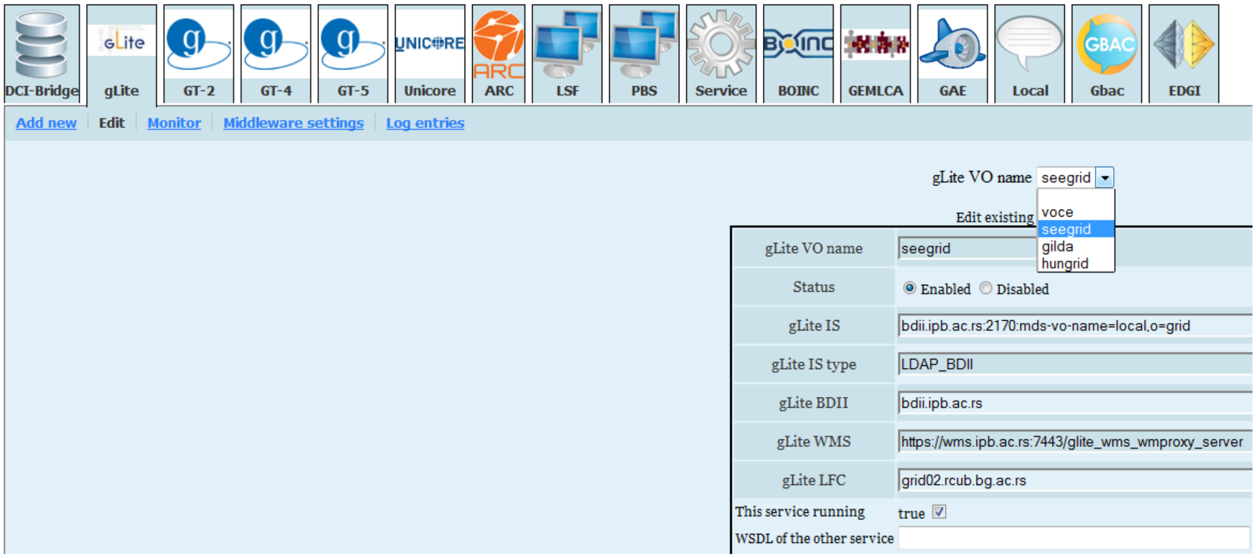
Figure 6.3 You can find detailed information about the VOs resource allocation and usage on the *GStat 2.0* linked on the top of gLite page

The gLite infrastructure is the most popular and widest used middleware in the EGI (former EGEE) community. The resources belonging to this middleware group are called Virtual Organizations and have the following central services which must reach:

- gLite BDII (information broadcasting server of the given VO)
- gLite WMS (arrival point to receive jobs in the given VO)
- gLite LFC (server for mapping the name/storage relations of remote grid files within the given VO)

---

[1] About supported resources you find more detailes descriptions in DCI Bridge Administrator Manual



gLite VO name: seegrid

Edit existing

gLite VO name	seegrid
Status	● Enabled ○ Disabled
gLite IS	bdii.ipb.ac.rs:2170:mds-vo-name=local,o=grid
gLite IS type	LDAP_BDII
gLite BDII	bdii.ipb.ac.rs
gLite WMS	https://wms.ipb.ac.rs:7443/glite_wms_wmproxy_server
gLite LFC	grid02.rcub.bg.ac.rs
This service running	true ☑
WSDL of the other service	

Figure 6.4 The supported gLite VOs and the properties of selected “seegrid” VO

The names of referenced VO-s will appear on the proper WS-PGRADE/Information/Resources/gLite menu (See Figure 6.4). The URL-s of the central services of the given VO will be visible when user selects one among the enumerated VO-s. This VO-s can be selected as Grids. See Figure 13 Part A gLite Submitter. The CE within the user selected VO - where the job will be executed - will be determined by late binding, more exactly by the brokering service of the given VO. However the user can modify the decision of the broker by proper setting of the JDL editor. (See JDL/RSL tab on Figure 13 Part A gLite Submitter). Proxy certificates are used for gLite job submission authorization. The user can gain proxy certificate by the help of the Certificate menu.

6.2.2 Local

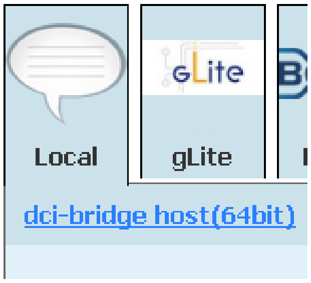


Figure 6.5 The WS-PGRADE/Information/Resources/Local menu

The *Local* resource is a distinguished one. The jobs submitted to a local resource will be not submitted on a remote resource (in the "Grid") but they will be executed within the gUSE infrastructure. See Figure 13 Part I for the job configuration. It burdens the limited resources: may spoil the overall throughput capacity of the gUSE therefore its usage is not suggested in public portals, and due restraint is recommended even at sporadic use.

Warning: The usage of local submitter is permitted in default case. The local submitter is permitted in default case after installation of system for initial testing at local level. However, it is strictly recommended for testing environment because of security aspects. Therefore the recommended status of local submitter is the "*Disabled*" for users after testing process. The usage of local submitter is not recommended in production level only for testing environments. Otherwise, it imposes a security hole. (Disable this plugin as soon as possible as it allows every user to gain full administrator access of the portal including access to private keys of certificates, database passwords and confidential user data.)

6.2.3 Web Services

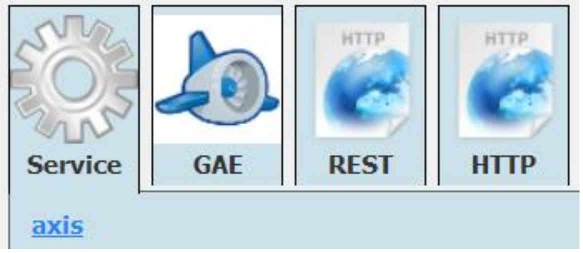


Figure 6.6 The only permitted web service: axis

The user can define any axis driven web service access during job configuration. See Appendix Figure 15.

6.2.4 Google App Engine (GAE)

The using of GAE is similar to **REST** and **HTTP** resources in gUSE/WS-PGRADE. (See chapter 6.2.17)

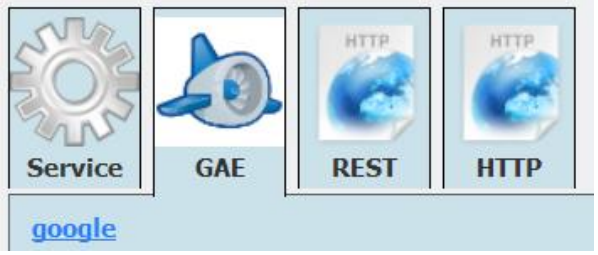
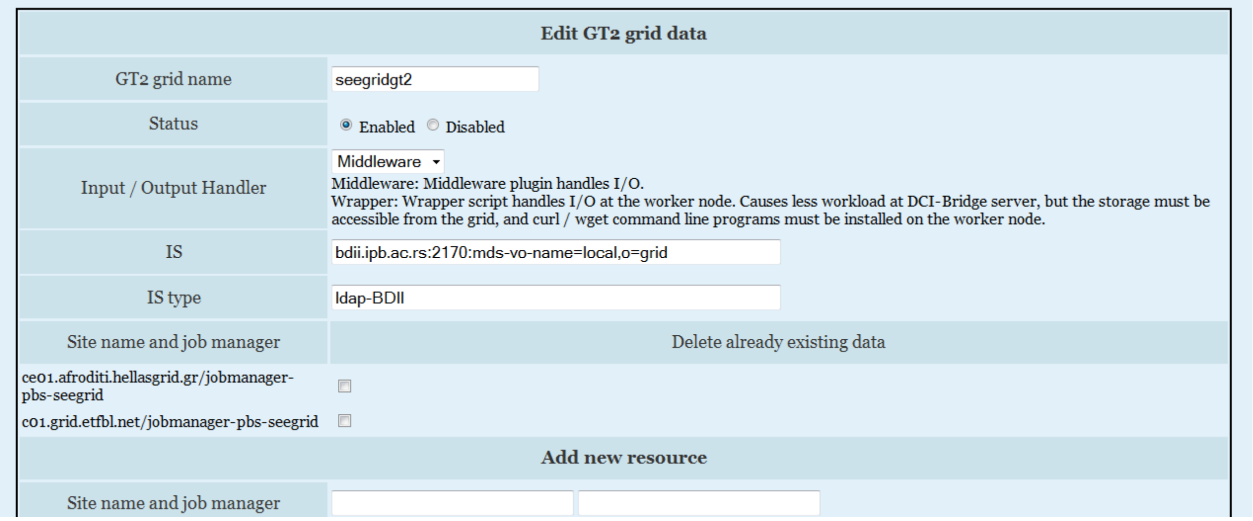


Figure 6.7 GAE with google service

6.2.4 GT2 (Globus Toolkit 2)



Edit GT2 grid data

GT2 grid name	seegridgt2
Status	● Enabled ○ Disabled
Input / Output Handler	Middleware Middleware: Middleware plugin handles I/O. Wrapper: Wrapper script handles I/O at the worker node. Causes less workload at DCI-Bridge server, but the storage must be accessible from the grid, and curl / wget command line programs must be installed on the worker node.
IS	bdii.ipb.ac.rs:2170:mds-vo-name=local,o=grid
IS type	ldap-BDII
Site name and job manager	Delete already existing data
ce01.afroditi.hellasgrid.gr/jobmanager-pbs-seegrid	☐
c01.grid.etfbl.net/jobmanager-pbs-seegrid	☐

Add new resource

Site name and job manager	

Figure 6.8 Defined sites of the selected Globus2 Grid Seegrid

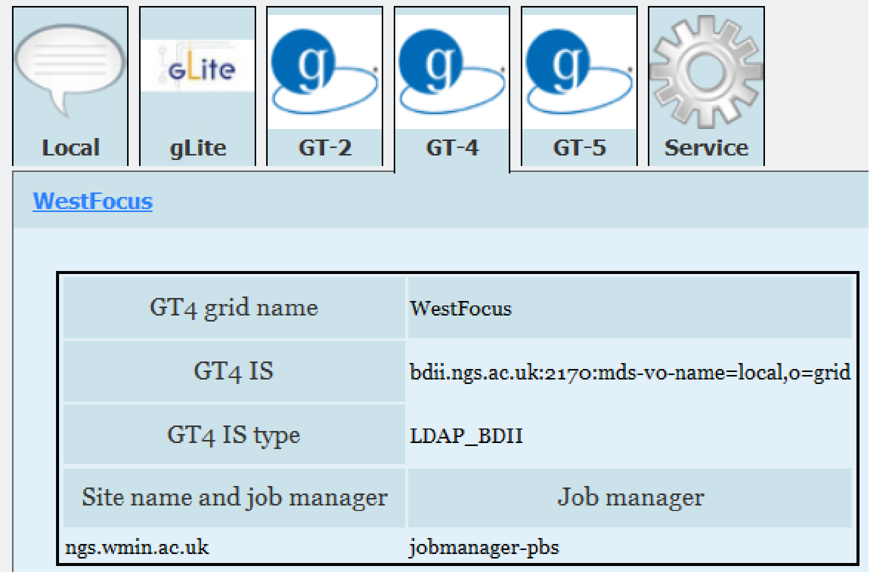
The menu lists the defined Globus2 Grids (There are one GT2 grids shown on the Figure 6.8: the GT2 services of the "seegridt2"). These Grids are associations of site bound resources. There are information systems from where information about the actually connected sites (with gLite terminology Computing Elements) can be gained. The System Administrator may add such sites to the given Globus2 Grid via the DCI-Bridge. The elements of the grid can be used as execution sites of jobs defined during job configuration.

A site is defined by two parameters:

1. *Site name* is the URL of the host machine representing header of the cluster implementing the given cluster.
2. *Job manager* is additional information for the resource bound job scheduler about the priority level of the job.

It follows that different resource items may be defined with common site but with different job-managers. During job configuration the site can be selected in the field Resource and the user can select among defined priority queues in the argument of *Job Manager*. See Figure 13 Part B - *gt2* submitter. Proxy certificates are used for *gt2* job submission authorization. The user can gain proxy certificate by the help of the *Certificate* menu.

6.2.6 GT4 (Globus Toolkit 4)



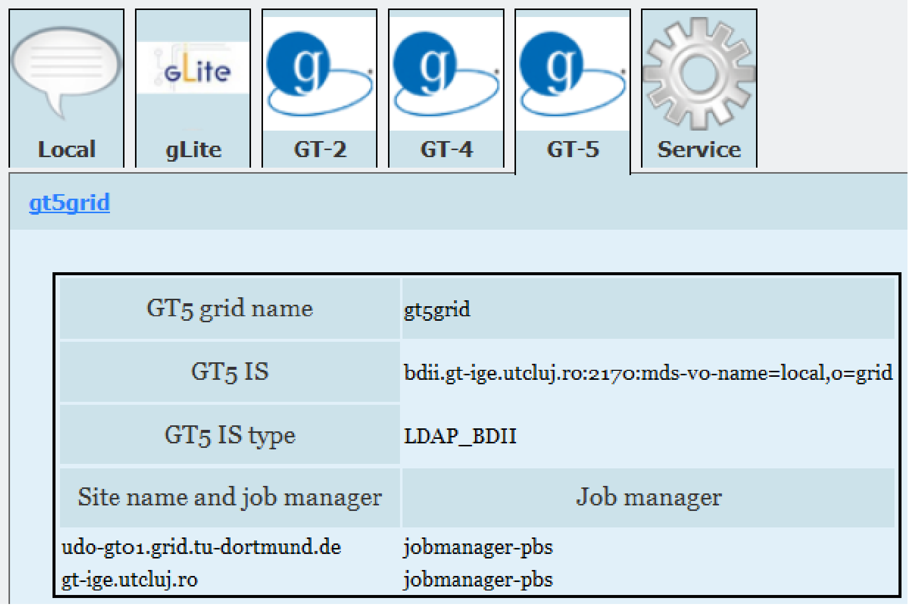
WestFocus

GT4 grid name	WestFocus
GT4 IS	bdii.ngs.ac.uk:2170:mds-vo-name=local,o=grid
GT4 IS type	LDAP_BDII
Site name and job manager	Job manager
ngs.wmin.ac.uk	jobmanager-pbs

Figure 6.9 Defined resources of the WestFocus grid which is based on GT4

GT4 is a successor technology of GT2. The usage of the tab is same as GT2 (See 6.2.5)

6.2.7 GT5 (Globus Toolkit 5)



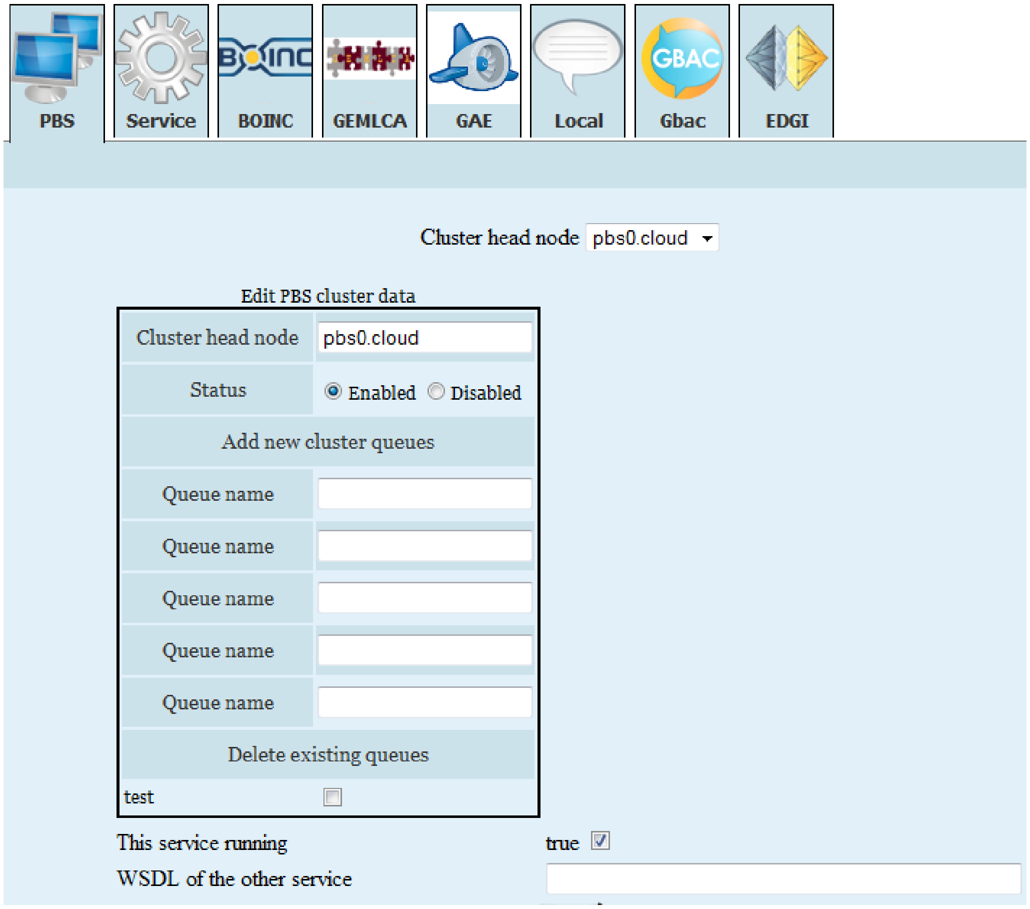
gt5grid

GT5 grid name	gt5grid
GT5 IS	bdii.gt-ige.utcluj.ro:2170:mds-vo-name=local,o=grid
GT5 IS type	LDAP_BDII
Site name and job manager	Job manager
udo-gt01.grid.tu-dortmund.de	jobmanager-pbs
gt-ige.utcluj.ro	jobmanager-pbs

Figure 6.10 Defined resources of the gt5grid which is based on GT5

GT5 is the last Globus grid type based on GT2 and works as same as the GT2 grid type (See 6.2.5).

6.2.8 PBS



Cluster head node pbs0.cloud

Edit PBS cluster data

Cluster head node	pbs0.cloud
Status	● Enabled ○ Disabled
Add new cluster queues	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Delete existing queues	
test	☐

This service running true ☑

WSDL of the other service

Figure 6.11 The PBS resource "pbs0.cloud" with queue definition options

LSF, SGE[2] and **PBS** are discussed together because they are almost identical from the point of view of the user. In both cases dedicated remote clusters are to be reached, where the jobs arrive in one of the defined priority queues of the given cluster. It is assumed that receiver resources already know the - portal generated - public key (and DN) of the user who sends the job. (See also the tab *Security/Public Key*). In this case the authorization happens by SSL upon the DN of the user which travels together with the job. There is only one accessible PBS cluster shown on Figure 6.11, the "pbs0.cloud". The jobs to this resource can be put in any of the tree defined priority queues. See *Appendix Fig. 13 Part F* for the job configuration.

About the role of LSF and PBS within the Public key handling function (in Public key menu) of WS-PGRADE you read in chapter 12 of Menu-Oriented Online Help.

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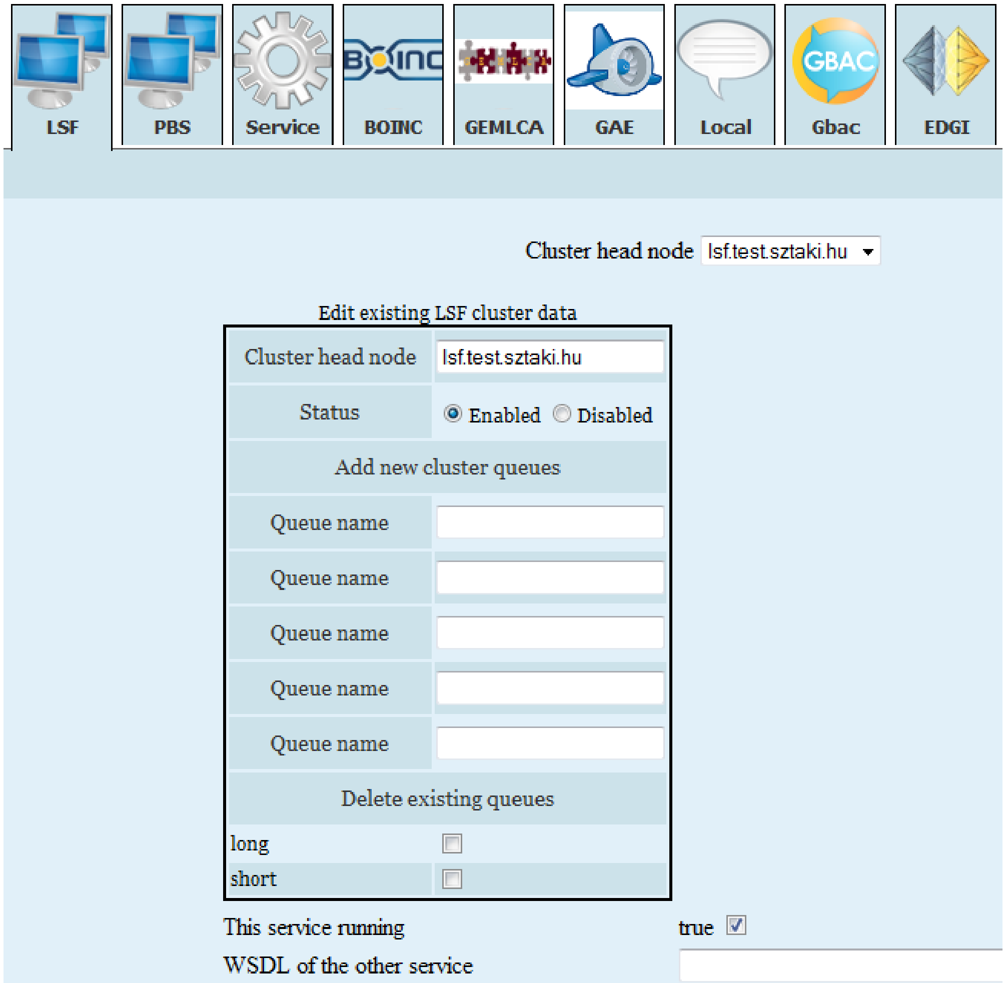
[2] The SGE plugin development comes from the gUSE Community (exactly from Optoelectronics and Visualisation Laboratory of Ruđer Bošković Institute, Zagreb). If you have further questions, please send it to Davor Davidovic (Davor.Davidovic@irb.hr).

6.2.9 LSF



Cluster head node lsf.test.sztaki.hu ▾

Edit existing LSF cluster data

Cluster head node	lsf.test.sztaki.hu
Status	● Enabled ○ Disabled
Add new cluster queues	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Delete existing queues	
long	☐
short	☐

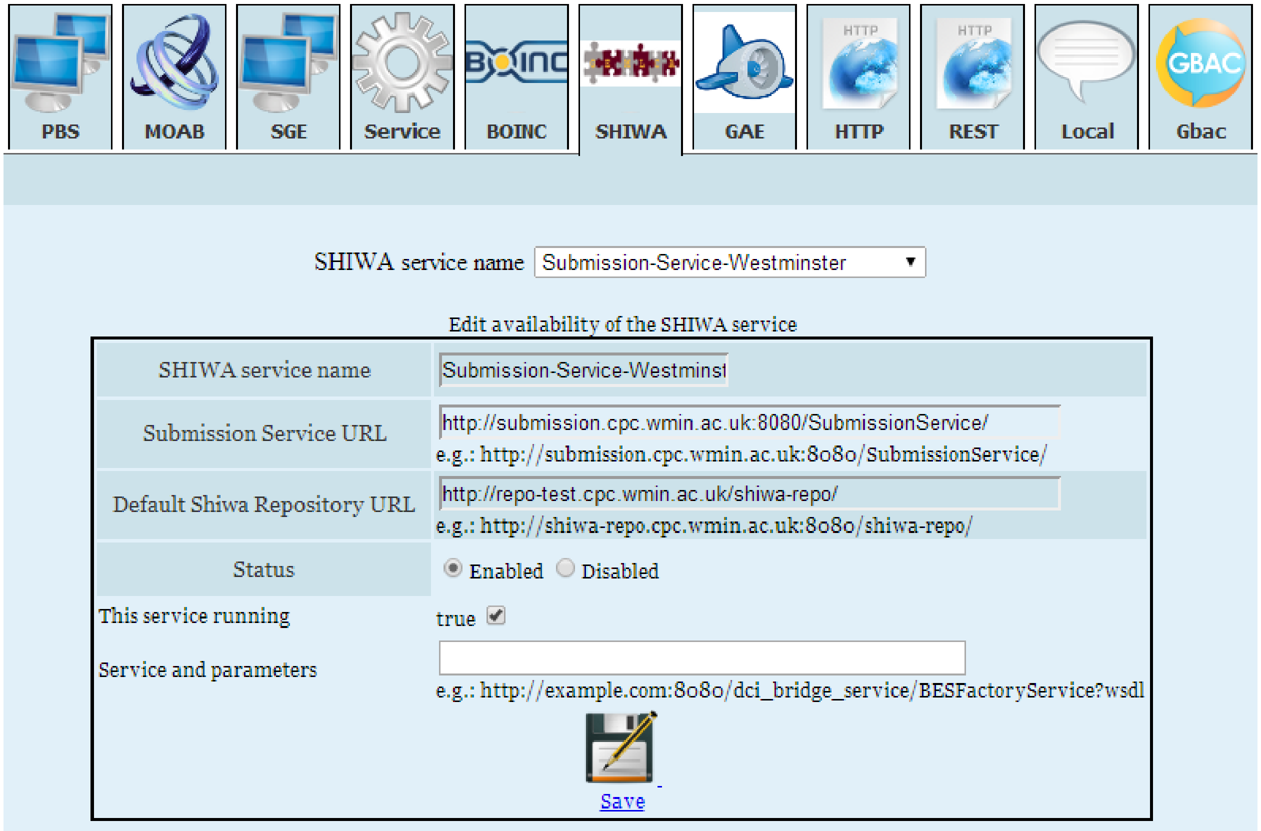
This service running true ☑

WSDL of the other service

Figure 6.12 The LSF resource "lsf.test.sztaki.hu" with queue definition options

LSF, SGE and PBS are discussed together (see 6.2.8). About the role of LSF and PBS within the *Public key* handling function (in Public key menu) of WS-PGRADE you read in chapter 12 of Menu-Oriented Online Help.

6.2.10 SHIWA



SHIWA service name: Submission-Service-Westminster ▾

Edit availability of the SHIWA service

SHIWA service name	Submission-Service-Westminst
Submission Service URL	http://submission.cpc.wmin.ac.uk:8080/SubmissionService/ e.g.: http://submission.cpc.wmin.ac.uk:8080/SubmissionService/
Default Shiwa Repository URL	http://repo-test.cpc.wmin.ac.uk/shiwa-repo/ e.g.: http://shiwa-repo.cpc.wmin.ac.uk:8080/shiwa-repo/
Status	● Enabled ○ Disabled
This service running	true ☑
Service and parameters	e.g.: http://example.com:8080/dci_bridge_service/BESFactoryService?wsdl

Figure 6.13 One SHIWA service in SHIWA repository

SHIWA is a special type of web services enabling the execution of legacy applications within their unmovable environments. The SHIWA service has a full introspection (self-exploring) facility therefore only the root access to an existing SHIWA repository (server) must be defined in the DCI Bridge. SHIWA resources which are interfaces to distinguished set of legacy applications have an own run time lookup system.

Warning: This look up system can be used if the user has a valid proxy certificate acceptable by the resource being questioned.

The look up system is used in two environments of the WS-PGRADE:

- **SHIWA Explorer menu**
- **Job Configuration** at SHIWA Job Executable (Appendix Figure 14) and SHIWA Port (Appendix Figure 19) configuration.

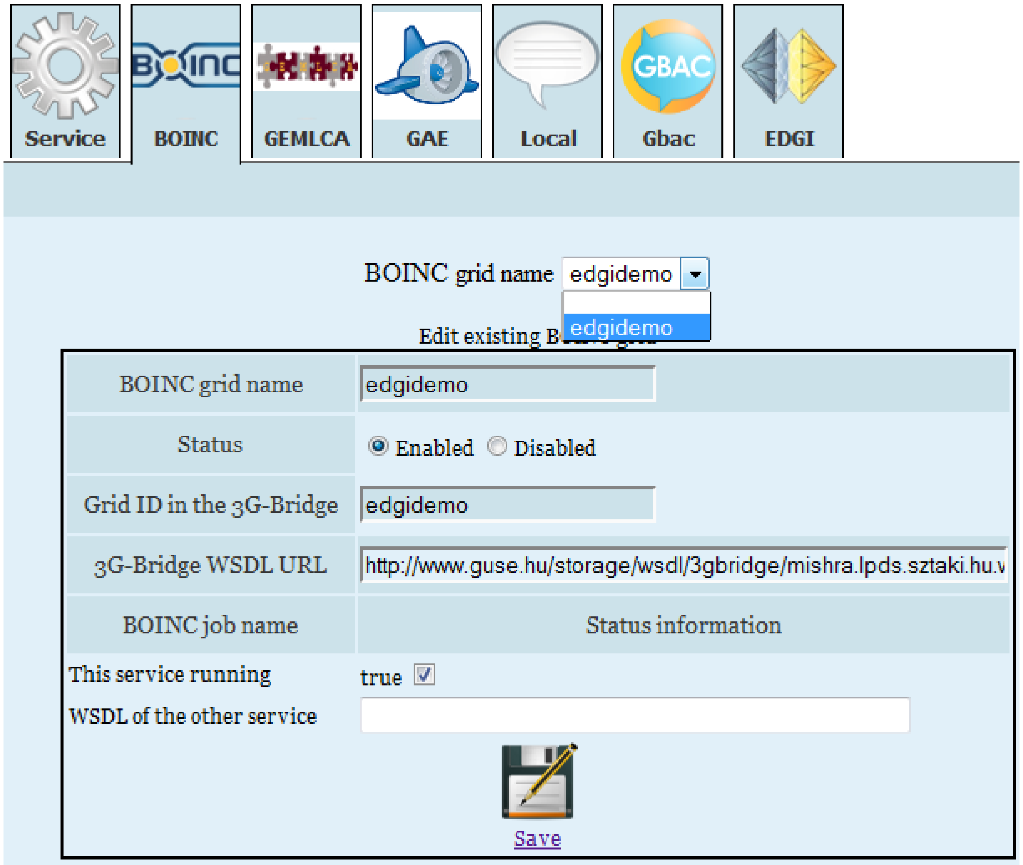
See detailed description about SHIWA-based job configuration in *chapter 23* within *Menu-Oriented Online Help*.

6.2.11 BOINC

The **BOINC** technology means a special way of application solving, where the given application have a (single) master (many) slave structure. A BOINC server stores the slave executables of the predefined applications. The slave executables may run on any of the client machines have been subscribed for the given application. The set of associated clients of a given BOINC server compose a BOINC Community. These communities can be regarded as grids, and they have a grid ID within a given BOINC Server.

As the 3G Bridge is a generic back end component of gUSE system it may host one or more BOINC servers.

Figure 6.14 lists the executable codes which can be executed on the client machines. A workflow job can be configured to select as BOINC Job one of the listed executables codes whose state is true. See Part D of Appendix Figure 13.



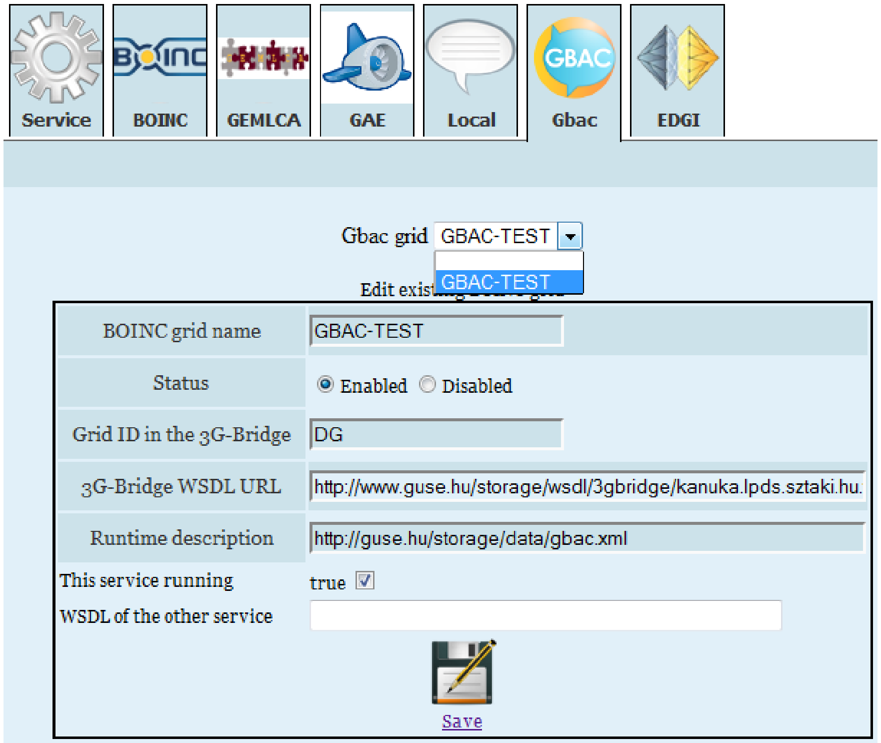
BOINC grid name edgidemo

Edit existing B

BOINC grid name	edgidemo
Status	● Enabled ○ Disabled
Grid ID in the 3G-Bridge	edgidemo
3G-Bridge WSDL URL	http://www.guse.hu/storage/wsdl/3gbridge/mishra.lpds.sztaki.hu.v
BOINC job name	Status information
This service running	true ☑
WSDL of the other service	

Figure 6.14 "Edgidemo" is the option in the BOINC-based grid list

6.2.12 GBAC



Gbac grid: GBAC-TEST

Edit exist

BOINC grid name	GBAC-TEST
Status	● Enabled ○ Disabled
Grid ID in the 3G-Bridge	DG
3G-Bridge WSDL URL	http://www.guse.hu/storage/wsdl/3gbridge/kanuka.lpds.sztaki.hu.
Runtime description	http://guse.hu/storage/data/gbac.xml
This service running	true ☑
WSDL of the other service	

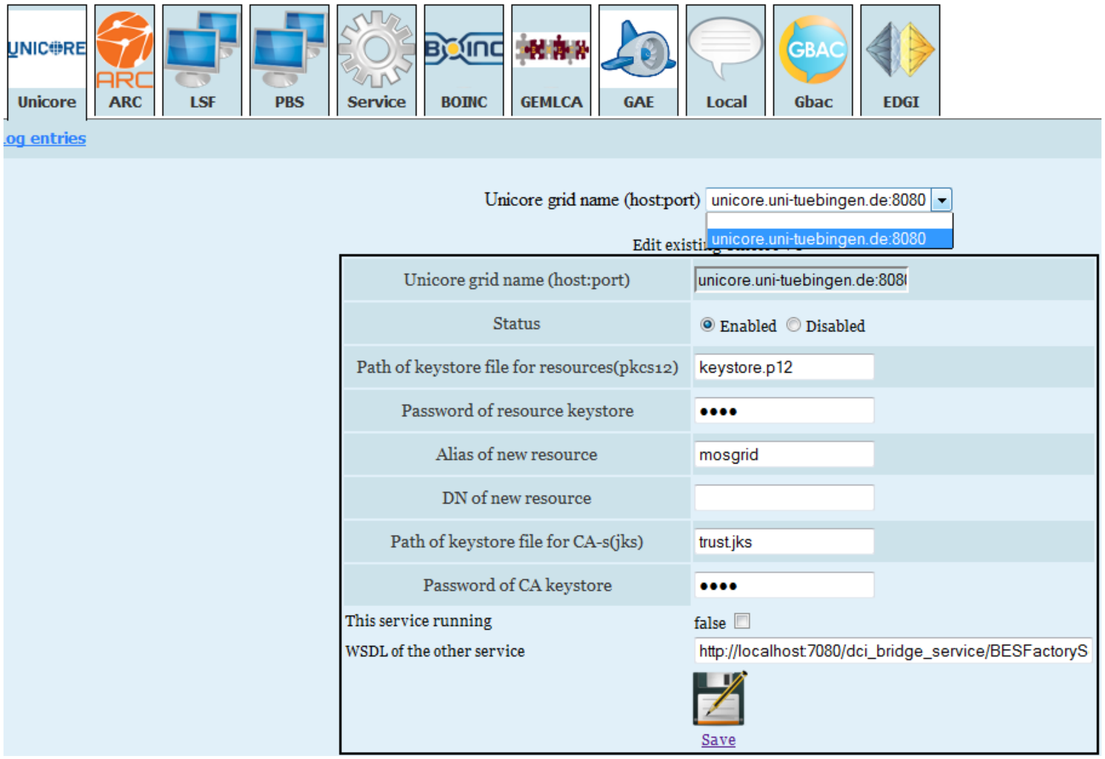
Figure 6.15 The details of the single GBAC type resource "gbac-test"

GBAC is a special variation of the BOINC technology (See chapter 6.2.11).

In the original BOINC the jobs to be executed must have a preinstalled executable on the BOINC server. In case of GBAC this executable will be replaced by a preinstalled computer image file. This image is able to execute the run time received job executable. Therefore slave machines of the BOINC community which are able to receive GBAC jobs must have a virtual execution enabled instruction set and must contain the Virtual Box application. The user can define an own executable - and not only one from a predefined list as in case of BOINC - in order to execute a code on a donated client machine of the selected Desktop Grid community. See the Workflow/Job Configuration: see Part E of Appendix Figure 13.

Note: If the job code executed on GBAC-based resource, the name extension for internal output prefix (where 0 <= index < n, and n is the number of generated generator output port files) is not happened. Therefore, it is not recommended to run a generator-type job on GBAC resource.

6.2.13 UNICORE



Unicore grid name (host:port) unicore.uni-tuebingen.de:8080

Edit existi

Unicore grid name (host:port)	unicore.uni-tuebingen.de:808
Status	● Enabled ○ Disabled
Path of keystore file for resources(pkcs12)	keystore.p12
Password of resource keystore	••••
Alias of new resource	mosgrid
DN of new resource	
Path of keystore file for CA-s(jks)	trust.jks
Password of CA keystore	••••
This service running	false ☐
WSDL of the other service	http://localhost:7080/dci_bridge_service/BESFactoryS

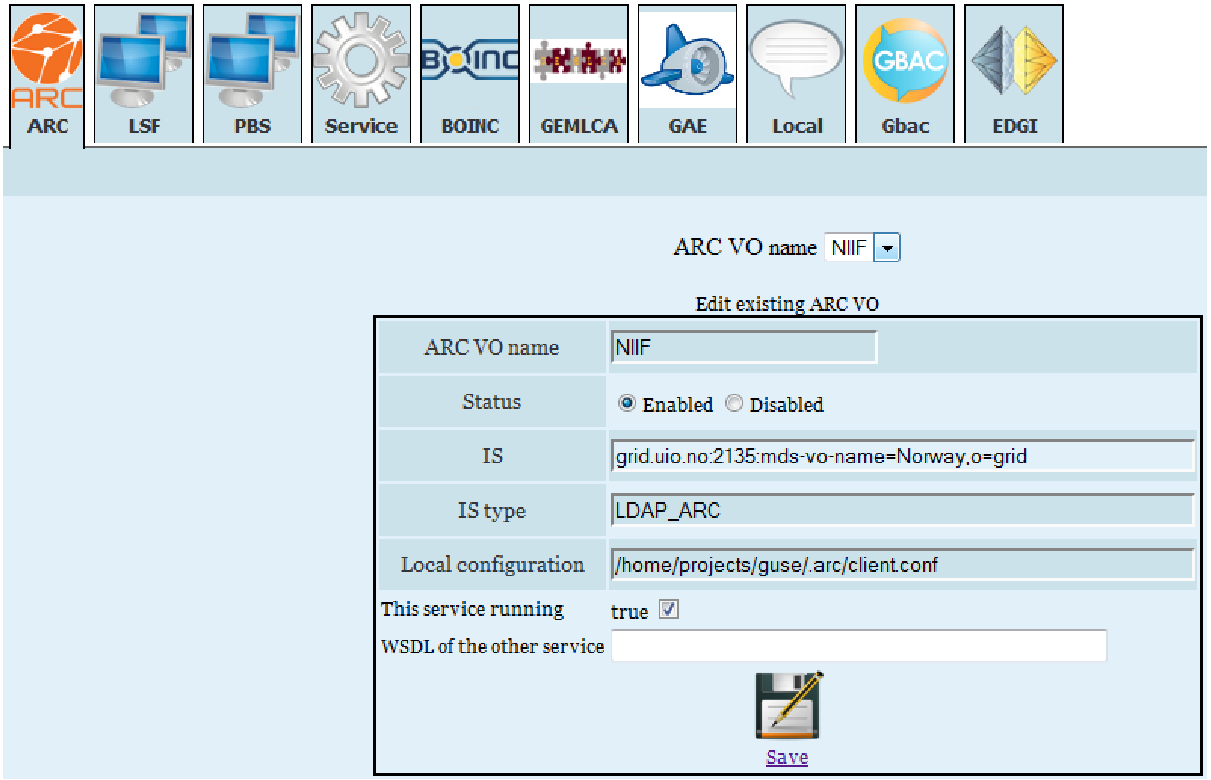
Figure 6.16 UNICORE resources: the Uni-Tuebingen is detailed

The UNICORE infrastructure is similar to GT2/GT5. The user may directly select among the accessible resources listed in Figures 6.16.

Warning: The "*Unicore grid name*" value should be set in format *<host:port>*. However, the so called *Assertion* file based technique is used instead of the MyProxy Server. The advantage of the Assertion technology is, that the user is not compelled to send her secrete key file through the network. See Part F of Appendix Figure 13 for the job configuration and the Assertion menu how to generate Assertion files.

Note: When using UNICORE try to avoid loading your certificate to the MyProxy Server via portal, use other methods such as CLI (Command Line Interface).

6.2.14 ARC



ARC VO name NIIF

Edit existing ARC VO

ARC VO name	NIIF
Status	● Enabled ○ Disabled
IS	grid.uio.no:2135:mds-vo-name=Norway,o=grid
IS type	LDAP_ARC
Local configuration	/home/projects/guse/.arc/client.conf
This service running	true ☑
WSDL of the other service	

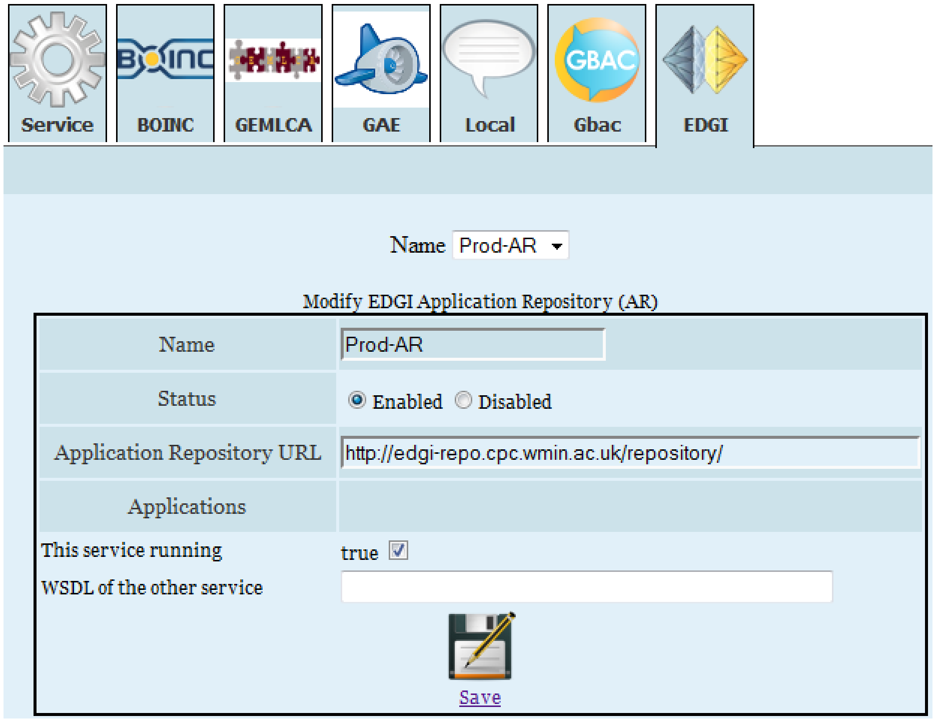
Figure 6.17 Details of the single reachable ARC based "NIIF" VO

ARC is the middleware of the NORDUGRID community. In some respect it is very similar to gLite. One main difference is that there is no central brokering service in ARC i.e. the client side defines the dedicated resource as the destination of the submission of her job. It uses proxy certificates as well.

Warning: However this proxy certificates must confirm to the newer RFC format. See the proper check box at the Upload page of the Certificate menu. See Part H of Appendix Figure 13 for the job configuration.

6.2.15 EDGI

EDGI (European Desktop Grid Initiative) middleware consolidates the extension of Service Grids with Desktop Grids (DGs) in order to support European Grid Initiative (EGI) and National Grid Initiative user communities that are users of Distributed Computing Infrastructures (DCIs) and require an extremely large number of CPUs and cores. By EDGI-based middleware support it is possible to use the Portal -> SG -> DG path (via DCI-Bridge) in order to run applications on the EDGI (SG -> DG) infrastructure. For using EDGI Application Repository (AR) to to run application, gUSE/WS-PGRADE supports the gLite DG resource type of EDGI infrastructure. Therefore, the reliable gLite VO certification method is necessary in this case, the gLite VO settings are needed by administrator in the job submission tool (e.g. in DCI-Bridge). (About EDGI job configuration, see chapter 16.)



Name Prod-AR

Modify EDGI Application Repository (AR)

Name	Prod-AR
Status	● Enabled ○ Disabled
Application Repository URL	http://edgi-repo.cpc.wmin.ac.uk/repository/
Applications	
This service running	true ☑
WSDL of the other service	

Figure 6.18 The "Prod-AR" is the only one EDGI VO name in EDGI resource type

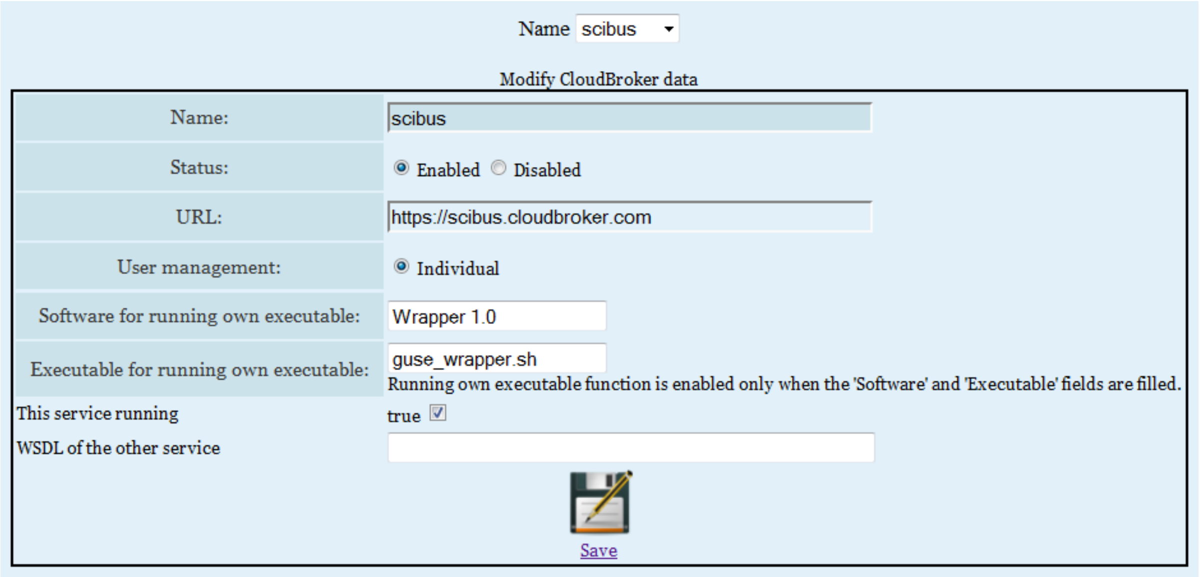
6.2.16 CB (CloudBroker)

The **CloudBroker (CB)** platform is an application store for high performance computing in the cloud. Through the CloudBroker menu of WS-PGRADE/gUSE different scientific and technical applications can be accessed, selected and immediately executed in the cloud, pay-per-use. Softwares (in cloud terminology: SaaS - Software as a Service) registered in the CB platform are stored in a repository, which can be queried by gUSE.

There is an opportunity to use the user her/his own executable binary code in CB job configuration process beside the selection of available software from CB repository. This new option is applicable by user if the corresponding software and executable names are set by DCI Bridge administrator to an application store in the DCI Bridge's Add new CloudBroker window (see Figure 40).

In order to work it, it needed previous to prepare an image in a cloud and create a new software that can run the user executable code over free resources defined in CB.

If the DCI Bridge receives a job for execution, and the selected application and software matches the ones set on the configuration interface, the user's provided custom executable is simply sent along with the job as an input file, where the application on a cloud (virtual machine) will arrange its execution. (About CB-job configuration see chapter 17.)


Name scibus

Modify CloudBroker data

Name:	scibus
Status:	● Enabled ○ Disabled
URL:	https://scibus.cloudbroker.com
User management:	● Individual
Software for running own executable:	Wrapper 1.0
Executable for running own executable:	guse_wrapper.sh Running own executable function is enabled only when the 'Software' and 'Executable' fields are filled.
This service running	true ☑
WSDL of the other service	

Figure 6.19 The details of the single CB type resource "scibus"

6.2.17 REST

REST stands for Representational State Transfer. It relies on a stateless, client-server, cacheable communications protocol - and in virtually all cases, the HTTP protocol is used. The REST applications use HTTP requests to post data (create and/or update), read data (e.g., make queries), and delete data. Thus, REST uses HTTP for all four **CRUD (Create/Read/Update/Delete)** operations. Much like Web Services, a REST service is:

- Platform-independent (you don't care if the server is Unix, the client is a Mac, or anything else),
- Language-independent (C# can talk to Java, etc.),
- Standards-based (runs on top of HTTP), and
- Can easily be used in the presence of firewalls.

The role and using of **GAE** and the **HTTP** resources is similar to REST in gUSE/WS-PGRADE (in all cases the core technology is the standard HTTP-based service messaging).

Note: The REST-based jobs (like the GAE- or HTTP-based jobs) you can configure as Services in WS-PGRADE.

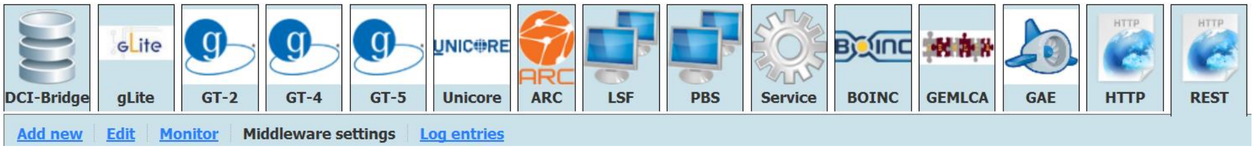


Figure 6.20 The menus related to REST resource – only the Monitor, Middleware settings, and Log entries functions are supported

6.2.18 HTTP

The role and using of **HTTP** resource is similar to **REST** in gUSE/WS-PGRADE. (see chapter 6.2.17)

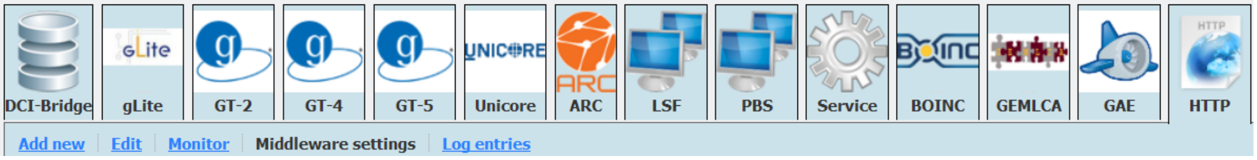


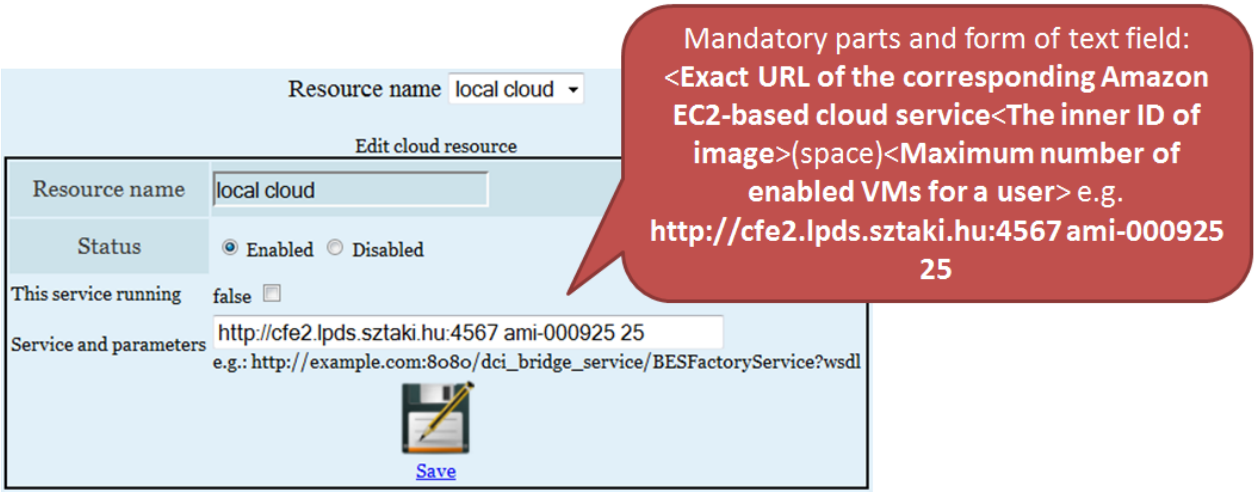
Figure 6.21 The menus related to HTTP resource – only the Monitor, Middleware settings, and Log entries functions are supported

6.2.19 Cloud (Amazon EC2 Cloud)

To use the **Cloud** resource it is needed to own exact authentication data to a cloud service that implements the **Amazon EC2** interface. This authentication data provides the cloud provider.

The solution behind the Cloud resource access stands the implementation of **Master** and **Slave DCI Bridge.** The Master DCI Bridge directly connects to gUSE forwards jobs through EC2-based frontend cloud service to the Slave DCI Bridge located in the cloud. Technically, the Master DCI Bridge starts by EC2-based service a Virtual Machine based on the previously created and saved image containing the properly configured Slave DCI Bridge. Since the Slave DCI Bridge is already configured and saved, you only need to configure the Master DCI Bridge.

Note: the Cloud middleware configuration is not differ from the configuration of a **Local** middleware – it is a **local cloud configuration**, essentially.



Mandatory parts and form of text field: **<Exact URL of the corresponding Amazon EC2-based cloud service<The inner ID of image>**(space)**<Maximum number of enabled VMs for a user>** e.g. **http://cfe2.lpds.sztaki.hu:4567 ami-000925 25**

Resource name local cloud

Edit cloud resource

Resource name	local cloud
Status	● Enabled ○ Disabled
This service running	false ☐
Service and parameters	http://cfe2.lpds.sztaki.hu:4567 ami-000925 25 e.g.: http://example.com:8080/dci_bridge_service/BESFactoryService?wsdl

Figure 6.22 The details of the Cloud resource editing

6.2.20 MOAB[3]

MOAB configuration and operation is very similar to PBS' and LSF'; please refer to section 6.2.8 to get detailed information about how to properly configure the MOAB submitter. However, the MOAB configuration screens offer a few extra options and we will discuss them in this section.

Serialize MOAB Access

Certain versions of MOAB have difficulties handling concurrent access. If access to a MOAB cluster is serialized, then all MOAB commands submitted from gUSE/WS-PGRADE to the head node will be serialized, that is, at no point in time will there be two concurrent command submissions to the same MOAB cluster. Serializing MOAB access can be thought of a simple workaround for MOAB versions that cannot handle concurrent access. Possible values: yes/no.

Cache Expiration

gUSE/WS-PGRADE polls the status of each of the submitted jobs. In order to minimize network access (each polling requires submitting a MOAB command via SSH), it is possible to cache job status. This setting sets the maximum number of milliseconds that each entry in the job status cache will have. Possible values: positive integer.

Error Tolerance Settings

Certain MOAB versions don't handle concurrency properly. Even if MOAB access is serialized, it is possible that MOAB commands can be submitted to the same MOAB cluster externally (i.e., via a shell terminal, outside WSPGRADE/gUSE). Under certain conditions external to WSPGRADE/gUSE, a submitted MOAB command could fail. The MOAB Submitter was designed to offer robust error tolerance.

---

[3] The MOAB plugin development comes from the gUSE Community (exactly from Applied Bioinfomatics Group of Eberhard Karls University, Tübingen). If you have further questions, please send it to Luis de la Garza (delagarza@informatik.uni-tuebingen.de).

Number of Attempts

This setting allows resubmission of a MOAB command in case it failed. A failed MOAB command will be resubmitted as many times as indicated in this settings. Possible values: positive integer.

Minimum Wait Time/Wait Time Window

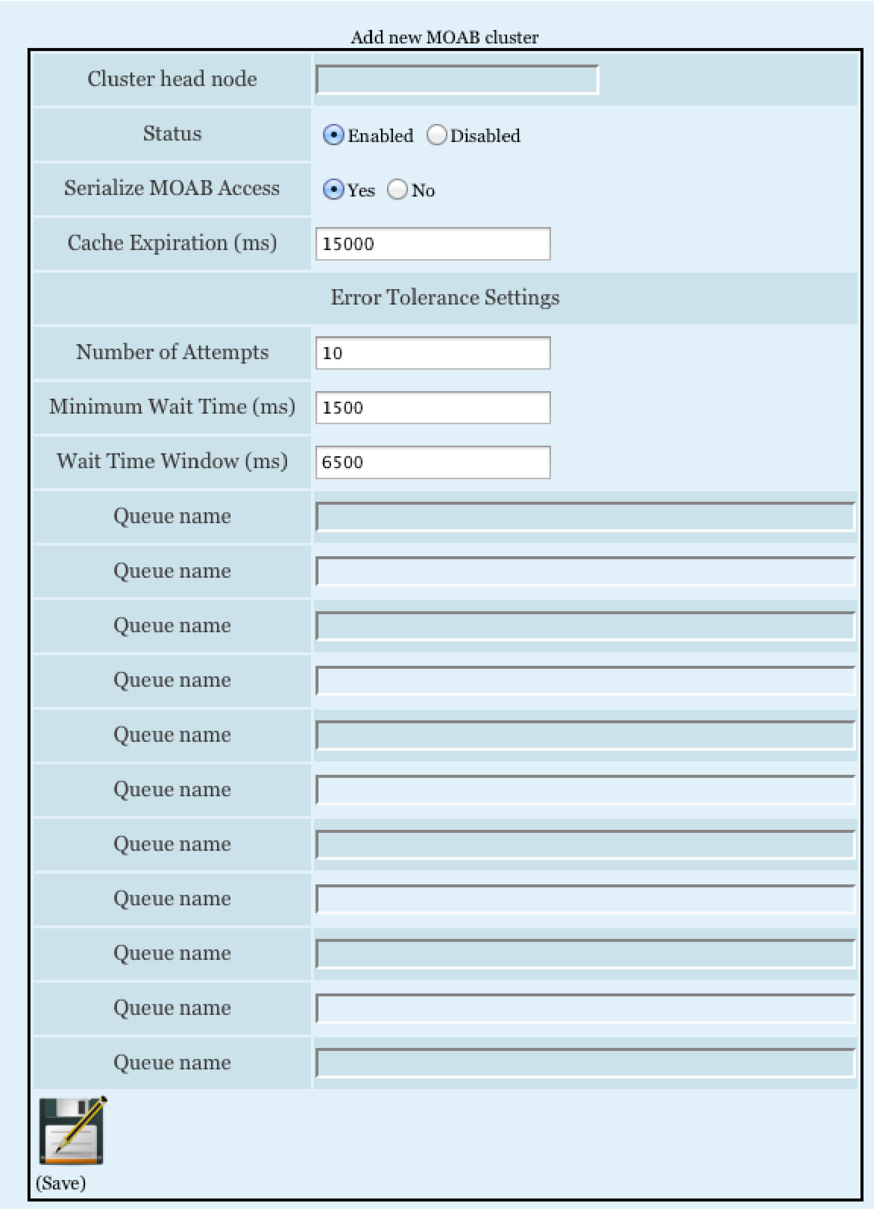
If the submission of a MOAB command fails, the MOAB Submitter will wait some time before attempting resubmission. If a command submission fails repeatedly, this time will increase. The formula for the waiting period between resubmissions is given by:

(attempts * min_wait_time) + (random * wait_window)

where:

- *attempts* - denotes the number of attempts that this particular command has been submitted.
- *min_wait_time* - the value, in milliseconds, given by the minimum wait time setting.
- *random* - represents a random number between zero and one, which is computed every time a resubmission is attempted.
- *wait_window* - the value, in milliseconds, given by the wait time window setting.

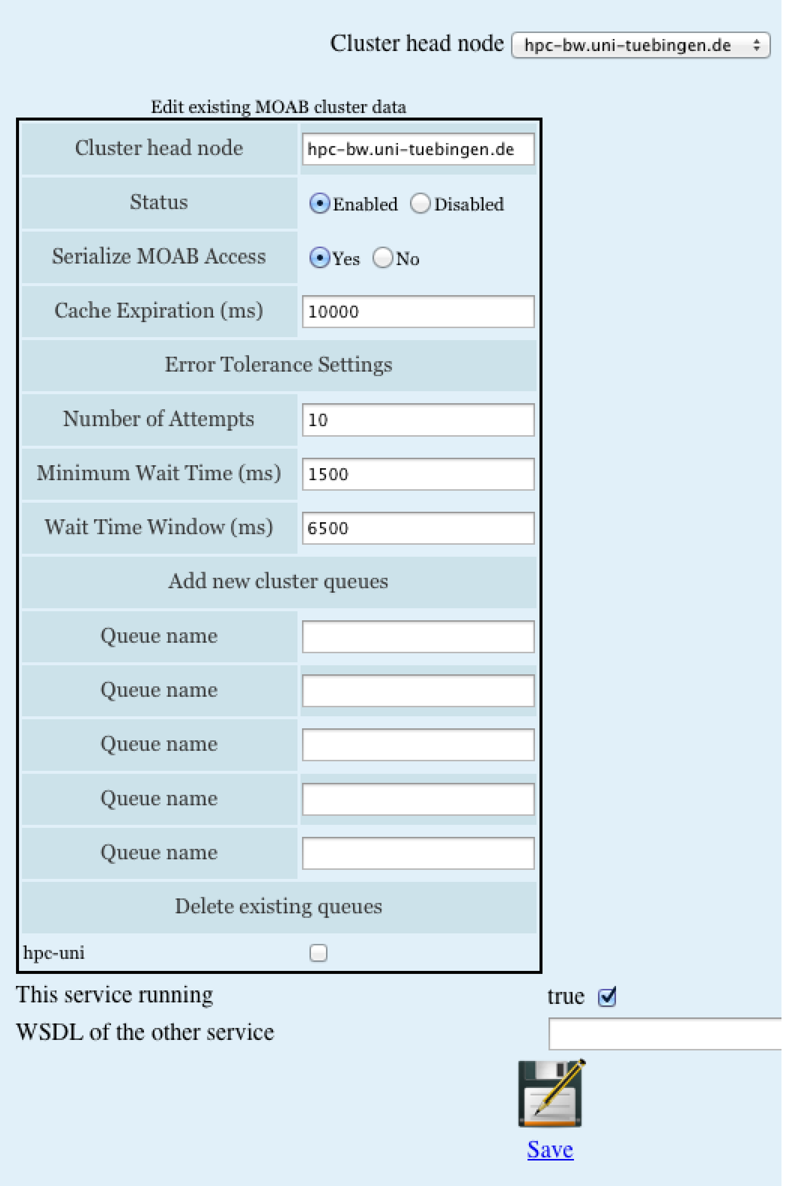
Thus we see that a minimum wait time is guaranteed and the more times a submission is attempted, the more time the MOAB Submitter will wait before attempting a resubmission. Possible values: positive integers.



Add new MOAB cluster

Cluster head node	
Status	● Enabled ○ Disabled
Serialize MOAB Access	● Yes ○ No
Cache Expiration (ms)	15000
Error Tolerance Settings	
Number of Attempts	10
Minimum Wait Time (ms)	1500
Wait Time Window (ms)	6500
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	

Figure 6.23 Adding new MOAB resource



Cluster head node hpc-bw.uni-tuebingen.de

Edit existing MOAB cluster data

Cluster head node	hpc-bw.uni-tuebingen.de
Status	● Enabled ○ Disabled
Serialize MOAB Access	● Yes ○ No
Cache Expiration (ms)	10000
Error Tolerance Settings	
Number of Attempts	10
Minimum Wait Time (ms)	1500
Wait Time Window (ms)	6500
Add new cluster queues	
Queue name	
Queue name	
Queue name	
Queue name	
Queue name	
Delete existing queues	
hpc-uni	☐

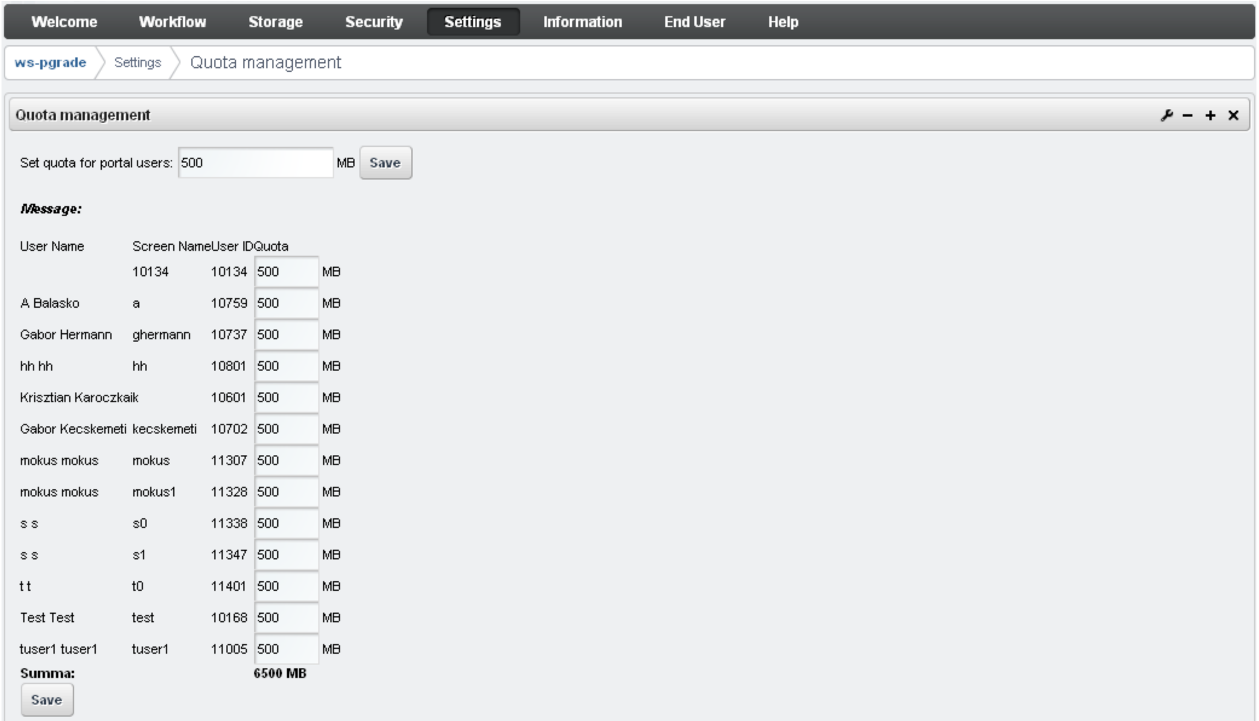
This service running true ☑

WSDL of the other service

Figure 6.24 Editing a MOAB resource

7. Quota Management – Only for System Administrators

Workflows, workflow related objects (graphs, templates) and first of all run time products of workflow instances are controlled by gUSE and - with the exception of input and output remote grid files – are stored in a common finite storage area. User storage quotas prevent the undue (accidental or malevolent) exhaustion of this precious resource. The quota allotted to a user is controlled by the system administrator via the *Quota management* menu:



Set quota for portal users: 500 MB

Message:

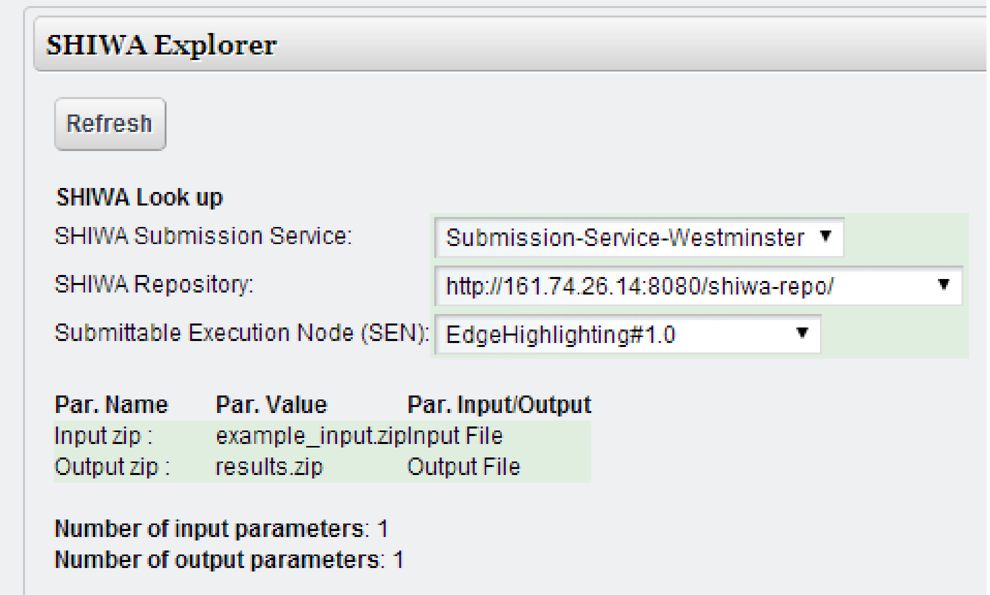
User Name	Screen Name	User ID	Quota	
	10134	10134	500	MB
A Balasko	a	10759	500	MB
Gabor Hermann	ghermann	10737	500	MB
hh hh	hh	10801	500	MB
Krisztian Karoczkaik		10601	500	MB
Gabor Kecskemeti	kecskemeti	10702	500	MB
mokus mokus	mokus	11307	500	MB
mokus mokus	mokus1	11328	500	MB
s s	s0	11338	500	MB
s s	s1	11347	500	MB
t t	t0	11401	500	MB
Test Test	test	10168	500	MB
tuser1 tuser1	tuser1	11005	500	MB
Summa:			**6500 MB**	

Figure 7.1 Quota management menu

Notes: The input field *Set quota for portal users* contains the default quota given to a new user. However the quota for each user can be reset individually. A user may get e-mail notification about the trespassing of own quota limit: see the Notification menu.

8. SHIWA Explorer

The runtime look up tool, **SHIWA Explorer** (*Information/SHIWA Explorer menu*) (See Fig. 8.1) helps you to find your desired executable (or in other words: legacy code) **Submittable Execution Node (SEN)** together with the related file parameters. Within a selected **SHIWA Submission Service** (a solution to submit legacy code located in a remote SHIWA Repository) and **SHIWA Repository** (a remote workflow repository) the available SENs are listed. Therefore, the SHIWA Explorer shows you the available SENs located in a SHIWA Repository that supports your portal's SHIWA Submission Service.



SHIWA Look up

SHIWA Submission Service: Submission-Service-Westminster

SHIWA Repository: http://161.74.26.14:8080/shiwa-repo/

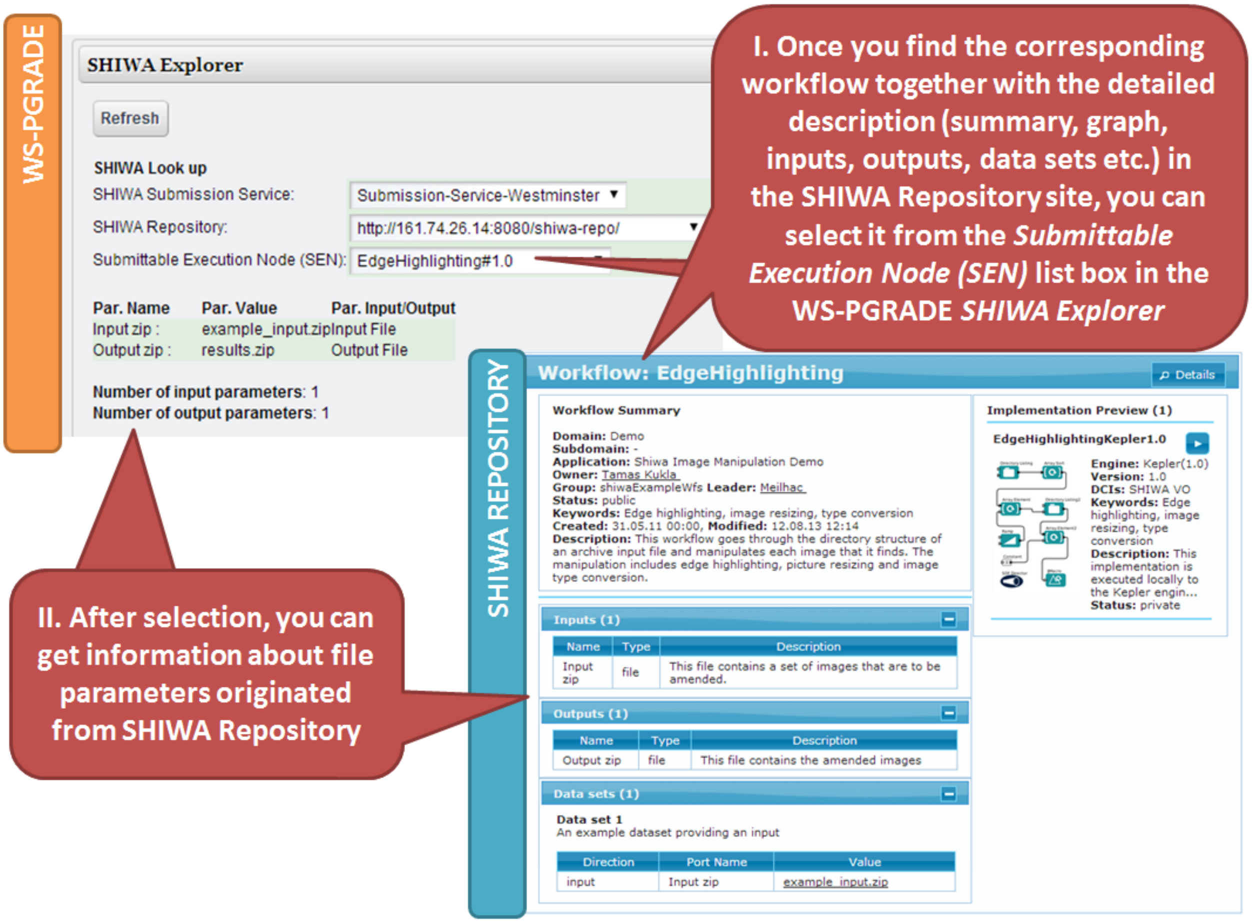
Submittable Execution Node (SEN): EdgeHighlighting#1.0

Par. Name	Par. Value	Par. Input/Output
Input zip :	example_input.zip	Input File
Output zip :	results.zip	Output File

Number of input parameters: 1
Number of output parameters: 1

Figure 8.1 The SHIWA explorer

Among the listed SENs you can search for your earlier saw one in the SHIWA Workflow Repository web site (http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/). Once you found it and selected it in the SHIWA Explorer, you get the whole file parameters of SEN (see Fig. 8.2). This information will be useful in the SHIWA-based workflow creation and configuration phase (see chapter 23 within Menu-Oriented Online Help).



SHIWA Explorer

SHIWA Look up

SHIWA Submission Service: Submission-Service-Westminster

SHIWA Repository: http://161.74.26.14:8080/shiwa-repo/

Submittable Execution Node (SEN): EdgeHighlighting#1.0

Par. Name	Par. Value	Par. Input/Output
Input zip :	example_input.zip	Input File
Output zip :	results.zip	Output File

Number of input parameters: 1
Number of output parameters: 1

I. Once you find the corresponding workflow together with the detailed description (summary, graph, inputs, outputs, data sets etc.) in the SHIWA Repository site, you can select it from the *Submittable Execution Node (SEN)* list box in the WS-PGRADE *SHIWA Explorer*

II. After selection, you can get information about file parameters originated from SHIWA Repository

Workflow: EdgeHighlighting

Workflow Summary

Domain: Demo
Subdomain: -
Application: Shiwa Image Manipulation Demo
Owner: Tamas Kukla
Group: shiwaExampleWfs **Leader:** Meilhac
Status: public
Keywords: Edge highlighting, image resizing, type conversion
Created: 31.05.11 00:00, **Modified:** 12.08.13 12:14
Description: This workflow goes through the directory structure of an archive input file and manipulates each image that it finds. The manipulation includes edge highlighting, picture resizing and image type conversion.

Implementation Preview (1)

EdgeHighlightingKepler1.0

Engine: Kepler(1.0)
Version: 1.0
DCIs: SHIWA VO
Keywords: Edge highlighting, image resizing, type conversion
Description: This implementation is executed locally to the Kepler engin...
Status: private

Inputs (1)

Name	Type	Description
Input zip	file	This file contains a set of images that are to be amended.

Outputs (1)

Name	Type	Description
Output zip	file	This file contains the amended images

Data sets (1)

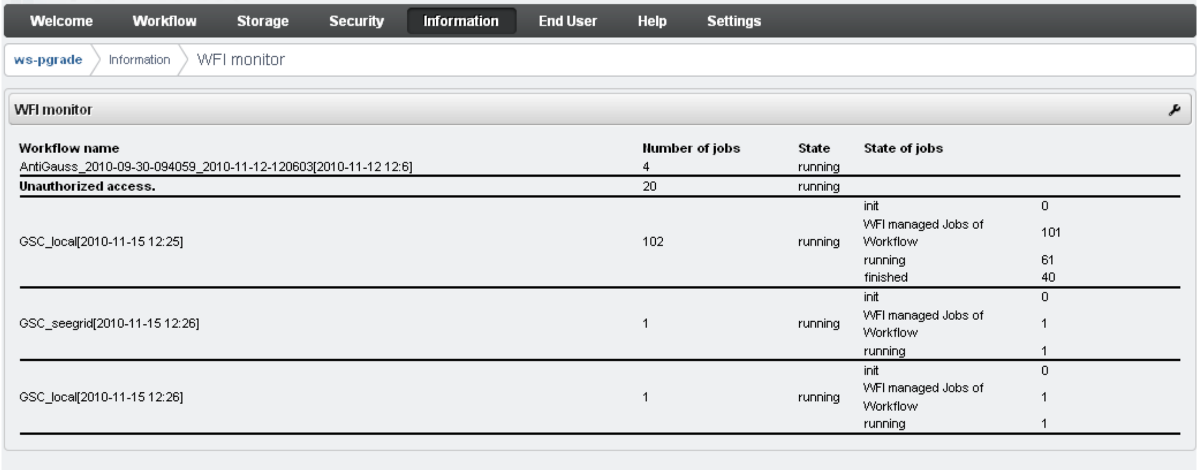
Data set 1
An example dataset providing an input

Direction	Port Name	Value
input	Input zip	example_input.zip

Figure 8.3 Input and Output parameters of the selected Submittable Execution Node (SEN)

9. WFI Monitor

The **WFI monitor** is the first and experimental test version of tools whose mission is the internal inspection of components constituting the gUSE. The WFI monitor collects run time statistics about the workflow interpreter component i.e. it is Component whose component type is "*wfi*".



Workflow name	Number of jobs	State	State of jobs	
AntiGauss_2010-09-30-094059_2010-11-12-120603[2010-11-12 12:6]	4	running		
Unauthorized access.	20	running		
GSC_local[2010-11-15 12:25]	102	running	init WFI managed Jobs of Workflow running finished	0 101 61 40
GSC_seegrid[2010-11-15 12:26]	1	running	init WFI managed Jobs of Workflow running	0 1 1
GSC_local[2010-11-15 12:26]	1	running	init WFI managed Jobs of Workflow running	0 1 1

Figure 9.1 WFI Monitor

The monitor lists a snapshot of the workflow instances handled by the "*wfi*" component(s) in the moment of the request. Within a workflow instance the states of job instances are discriminated and the accumulated numbers are displayed.

Notes:

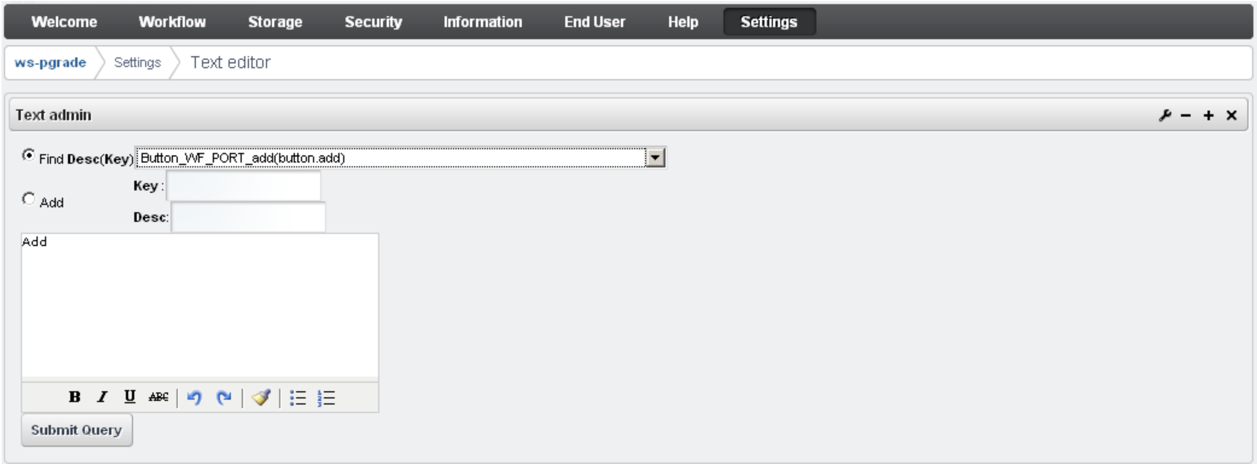
Only the workflow instances just being interpreted are displayed.

Submitted workflow instances of others users are displayed as well. However the names of foreign workflow instances are not displayed for because of privacy reasons, and substituted by the "*Unauthorized access*" text.

The system administrator user will have distinguished rights in the planned next release of the WFI Monitor: he/she can delete any workflow of any user clicking on the delete button associated in to each workflow.

10. Text Editor – Only for System Administrators

The system administrator may change displayed texts of portlets on such places where the JSP responsible for the layout of a portlet contains certain keys. The keys will be substituted by the associated text value. The key value pairs a stored in the central database of the gUSE system, and the key value record is maintained by the Text editor portlet. If there is no matching database item for a given key then the key string will be rendered by the JSP.



● Find Desc(Key) Button_WF_PORT_add(button.add)

○ Add

Add

Figure 10.1 Text editor menu

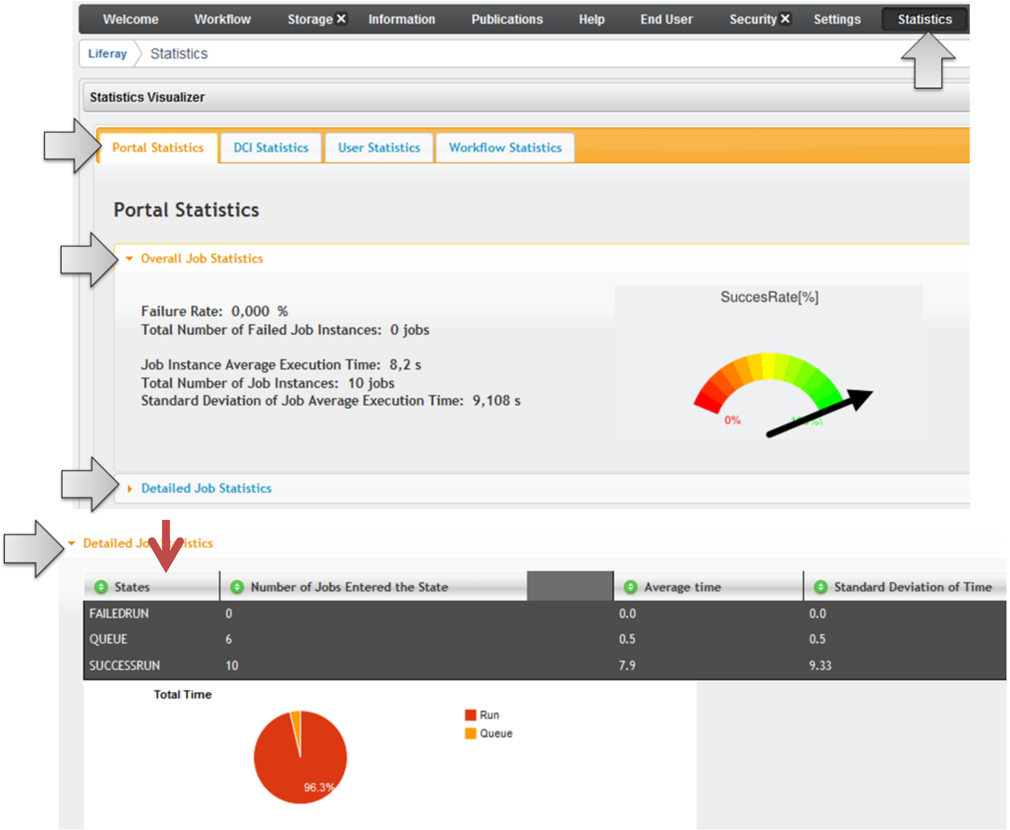
Notes:

New key-value items can be defined by selecting the *Add* radio button, filling the three input fields and confirming the operation by clicking the *Submit Query* button where the value entered for key: should match the key in the JSP; the *Descriptor* value is a free text entered in order to help the user to find the given item, and the unlabeled text area should contain the defined value text which will substitute the key during the rendering of the proper portlet.

An existing key-value item can be found (and its value eventually edited) selecting the *Find* radio button and using associated check list button. The items in this list are displayed such a way that the key in parentheses follows the descriptor. However the items in the list are enumerated in the lexicographical order of the key part.

11. Collection and Visualization of Usage Statistics

The **Statistics** function that is represents the collection and visualization of usage statistics in gUSE/WS-PGRADE is responsible for collecting and storing metrics in the database and for display of these metrics. This function allows viewing metrics in four tabs, portal, DCI, user, and workflow, on seven levels, portal, user, DCI, resource, concrete workflow, workflow instance and abstract job. This is accomplished by allowing users to navigate to different pages to see the level of statistics they want. This solution is helpful for administrator in resource settings (mainly from portal and DCI statistics) for user in middleware, resource selecting and in job execution time estimation (mainly from user and workflow statistics).


Welcome
Workflow
Storage ✕
Information
Publications
Help
End User
Security ✕
Settings
Statistics
Liferay
Statistics
Statistics Visualizer
Portal Statistics
DCI Statistics
User Statistics
Workflow Statistics
Portal Statistics
Overall Job Statistics
SuccesRate[%]
0%
Detailed Job Statistics
Detailed Job Statistics
Total Time
96.3%
Run
Queue

Failure Rate: 0,000 %
Total Number of Failed Job Instances: 0 jobs

Job Instance Average Execution Time: 8,2 s
Total Number of Job Instances: 10 jobs
Standard Deviation of Job Average Execution Time: 9,108 s

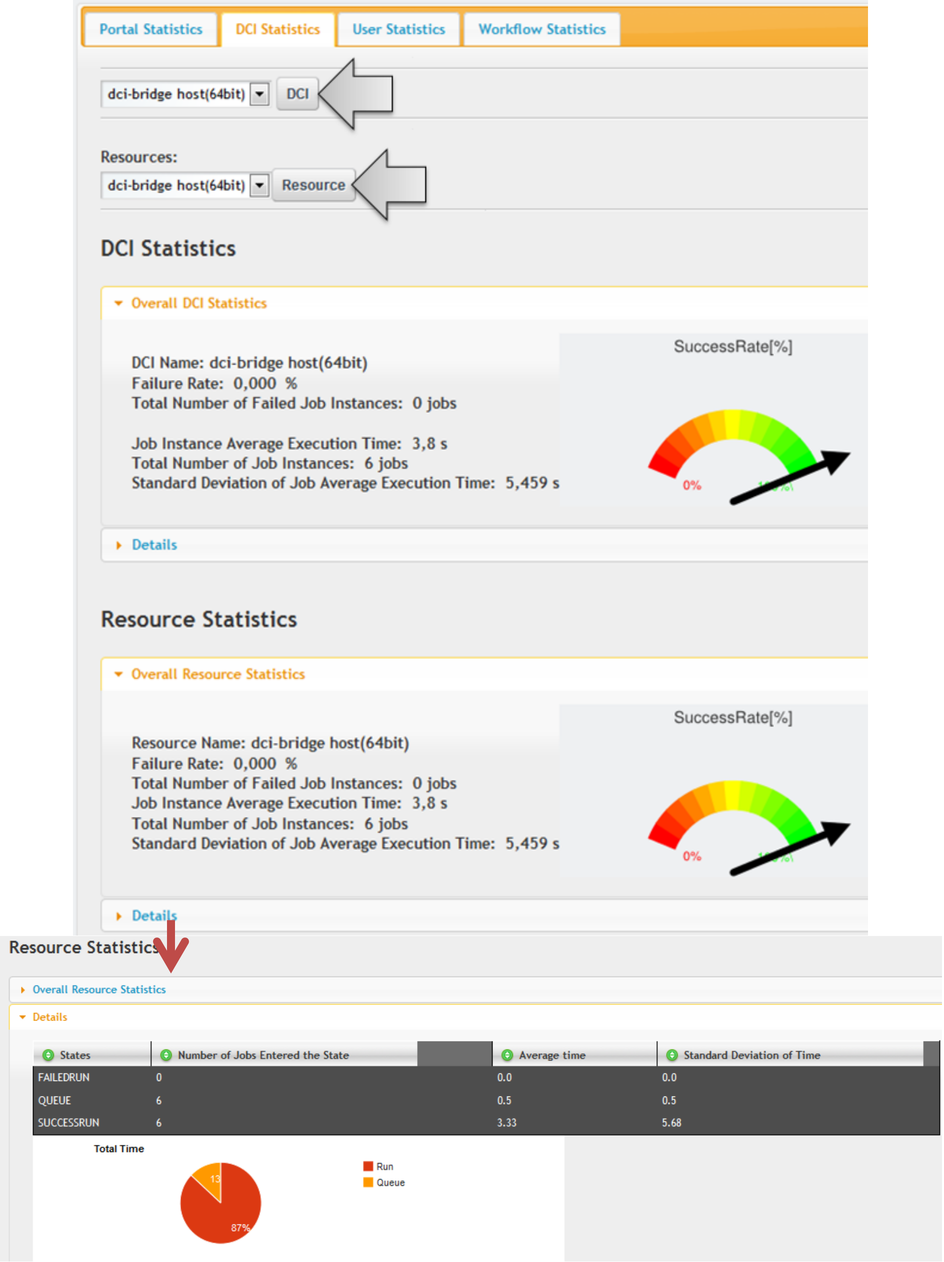
States	Number of Jobs Entered the State	Average time	Standard Deviation of Time
FAILEDRUN	0	0.0	0.0
QUEUE	6	0.5	0.5
SUCCESSRUN	10	7.9	9.33

Figure 11.1 The Portal Statistics tab with Overall Portal Statistics (above) and with Detailed Job Statistics (below) part

The default page view upon clicking the *Statistics* tab is the metrics for the portal (see Figure 11.1). The other pages, the *Portal Statistics, DCI Statistics, User Statistics, Workflow Statistics* can be accessed through tabs at the top of the page.

The first two tabs show a global view about portal and DCI for all users, while the other two tabs give useful information for the single users. The provided information is organized into two main parts, into overall statistics and details part. In the overall statistics area the user finds five figures about jobs in all cases: *Failure Rate, Total Number of Failed Job Instances, Job Instance Average Execution Time, Total Number of Job Instances,* and *Standard Deviation of Job Average Execution Time*.

Additionally, the success rate is expressed by graphical chart. (The job execution time means the time between the ready for submission status and the status of finished running.) In the details area (see also Figure 11.1) the user finds additional information about portal, DCI, user or workflow statistics in form of table and pie chart. The rows of tables consist of three potential job states, the queue (waiting for running), and the two possible result states of job running, the success run and the failed run. The columns of table give information about *Number of Jobs Entered the State*, the *Average Time* (expressed in seconds), and the *Standard Deviation of Time* (expressed in seconds) for each states. The pie chart in *Details* area shows the rate of run and queue times in total time.


Portal Statistics
DCI Statistics
User Statistics
Workflow Statistics
dci-bridge host(64bit)
DCI
Resources:
dci-bridge host(64bit)
Resource
DCI Statistics
Overall DCI Statistics
SuccessRate[%]
0%
Details
Resource Statistics
Overall Resource Statistics
SuccessRate[%]
0%
Details
Resource Statistics
Overall Resource Statistics
Details
Total Time
13
87%
Run
Queue

DCI Name: dci-bridge host(64bit)
Failure Rate: 0,000 %
Total Number of Failed Job Instances: 0 jobs

Job Instance Average Execution Time: 3,8 s
Total Number of Job Instances: 6 jobs
Standard Deviation of Job Average Execution Time: 5,459 s

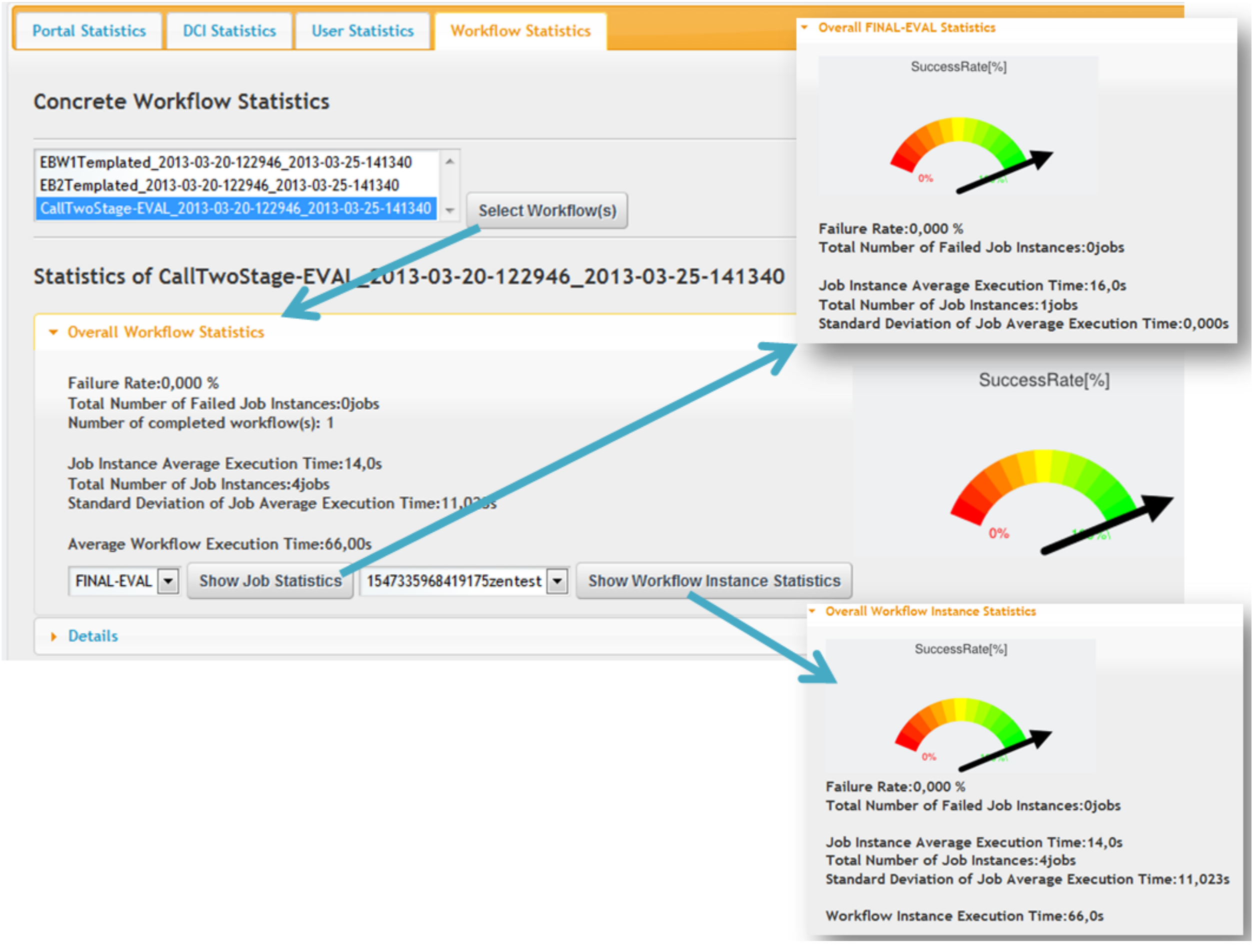
Resource Name: dci-bridge host(64bit)
Failure Rate: 0,000 %
Total Number of Failed Job Instances: 0 jobs
Job Instance Average Execution Time: 3,8 s
Total Number of Job Instances: 6 jobs
Standard Deviation of Job Average Execution Time: 5,459 s

States	Number of Jobs Entered the State	Average time	Standard Deviation of Time
FAILEDRUN	0	0.0	0.0
QUEUE	6	0.5	0.5
SUCCESSRUN	6	3.33	5.68

Figure 11.2 The DCI Statistics tab with Overall DCI Statistics (above) and with Details (below) part

The above-mentioned features concern for all tabs in the menu.

Let’s see now the four tabs with details. The *Portal Statistics* window (Figure 11.1) shows the above-mentioned metrics elements about the given portal. In *DCI Statistics* window are two list boxes for user to choose a *DCI* (the list box includes *dci bridge host (64 bit)* and *guse wfi*) and a *Resource* by clicking the *DCI* and *Resource* buttons (Figure 11.2). The result for the two type of selection appears separately and the detailed statistics with the well-known table and chart appears separately, too.



Concrete Workflow Statistics

EBW1Templated_2013-03-20-122946_2013-03-25-141340
EB2Templated_2013-03-20-122946_2013-03-25-141340
CallTwoStage-EVAL_2013-03-20-122946_2013-03-25-141340

Statistics of CallTwoStage-EVAL_2013-03-20-122946_2013-03-25-141340

Overall Workflow Statistics

Failure Rate:0,000 %
Total Number of Failed Job Instances:0jobs
Number of completed workflow(s): 1

Job Instance Average Execution Time:14,0s
Total Number of Job Instances:4jobs
Standard Deviation of Job Average Execution Time:11,023s

Average Workflow Execution Time:66,00s

FINAL-EVAL
1547335968419175zentest

Overall FINAL-EVAL Statistics

Failure Rate:0,000 %
Total Number of Failed Job Instances:0jobs

Job Instance Average Execution Time:16,0s
Total Number of Job Instances:1jobs
Standard Deviation of Job Average Execution Time:0,000s

Overall Workflow Instance Statistics

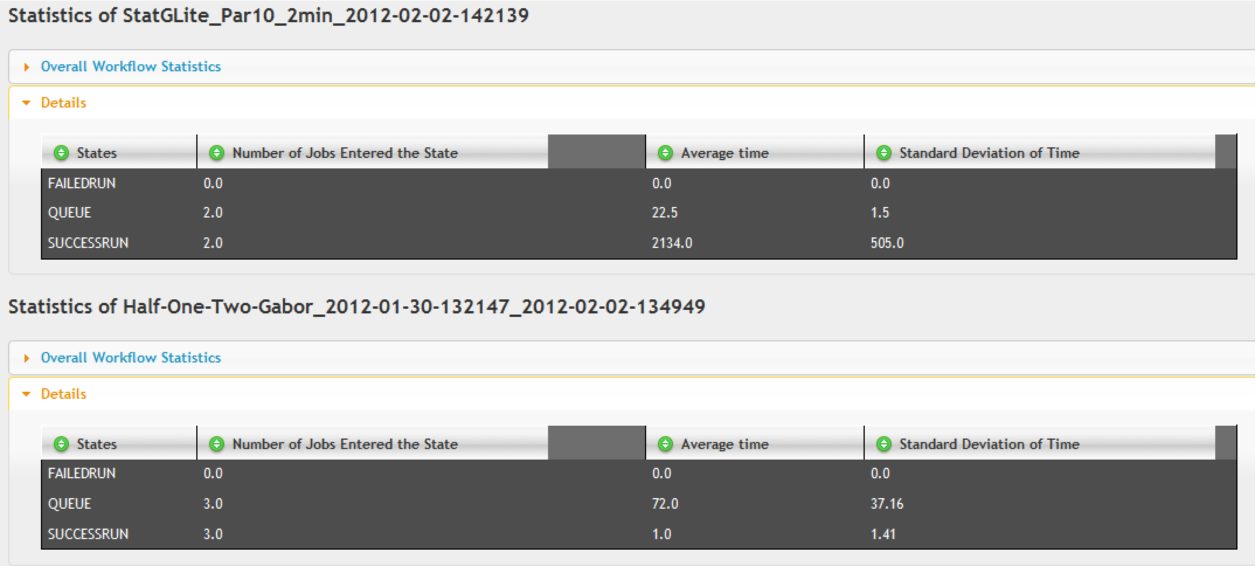
Failure Rate:0,000 %
Total Number of Failed Job Instances:0jobs

Job Instance Average Execution Time:14,0s
Total Number of Job Instances:4jobs
Standard Deviation of Job Average Execution Time:11,023s

Workflow Instance Execution Time:66,0s

Figure 11.3 The Workflow Statistics tab with Overall Workflow Statistics function

In the *User Statistics* tab the registered you can get data about her/his own activity, about the executed workflows and job instances. The visual structure of provided statistics is the same as in the *Portal Statistics* tab. Helpful information could be also retrieve from the last part of the menu statistics from the *Workflow Statistics* (Figure 11.3). Here you can select one or more concrete workflows by choosing an item from list box and then clicking *Select Workflow*(s) button. Then the *Overall Workflow Statistics* tab appears from where you can find the well-known five important statistical data about workflow jobs. Besides this data you can find here figures about *Number of completed workflow(s)* and about *Average Workflow Execution Time.* Additionally, you have opportunity to refine the statistics by choosing an item from lists and then clicking *Show Job Statistics* and *Show Workflow Instance Statistics* button. In the former case, at job statistics you get information about a job that may run in more workflow instances, while at workflow statistics the figures gives for users a picture about a workflow instance that comprises one or more job instances, sequentially. You can retrieve information about the running results of a job from the table of *Details* part of workflow statistics (Figure 11.4).



Statistics of StatGLite_Par10_2min_2012-02-02-142139

States	Number of Jobs Entered the State	Average time	Standard Deviation of Time
FAILEDRUN	0.0	0.0	0.0
QUEUE	2.0	22.5	1.5
SUCCESSRUN	2.0	2134.0	505.0

Statistics of Half-One-Two-Gabor_2012-01-30-132147_2012-02-02-134949

States	Number of Jobs Entered the State	Average time	Standard Deviation of Time
FAILEDRUN	0.0	0.0	0.0
QUEUE	3.0	72.0	37.16
SUCCESSRUN	3.0	1.0	1.41

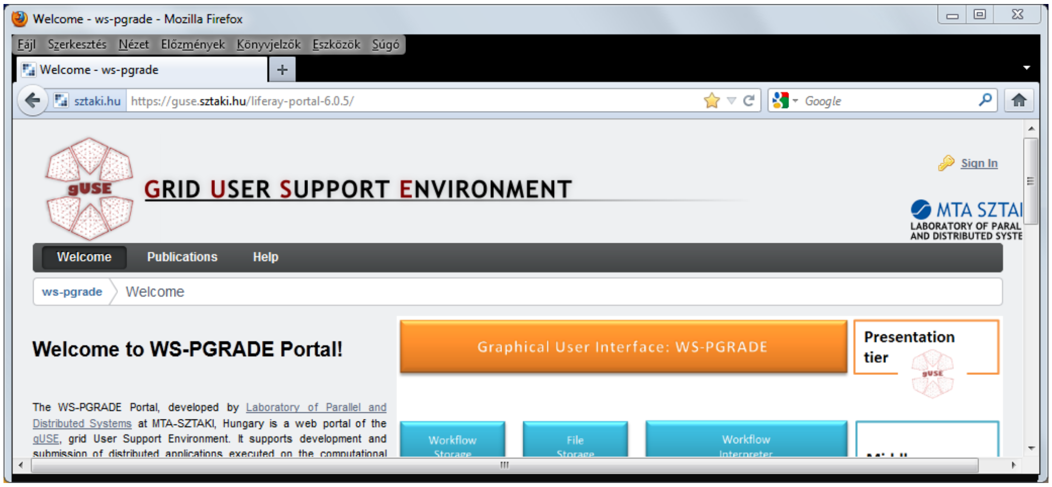
Figure 11.4 The Workflow Statistics tab with Overall Details in case of more concrete workflows selection

12. User Management

The main steps of user management process are the following:

1. Create a user account: (Depending on portal installation and security model the process may be different.)

1.1 Go to the portal (https://guse.sztaki.hu):

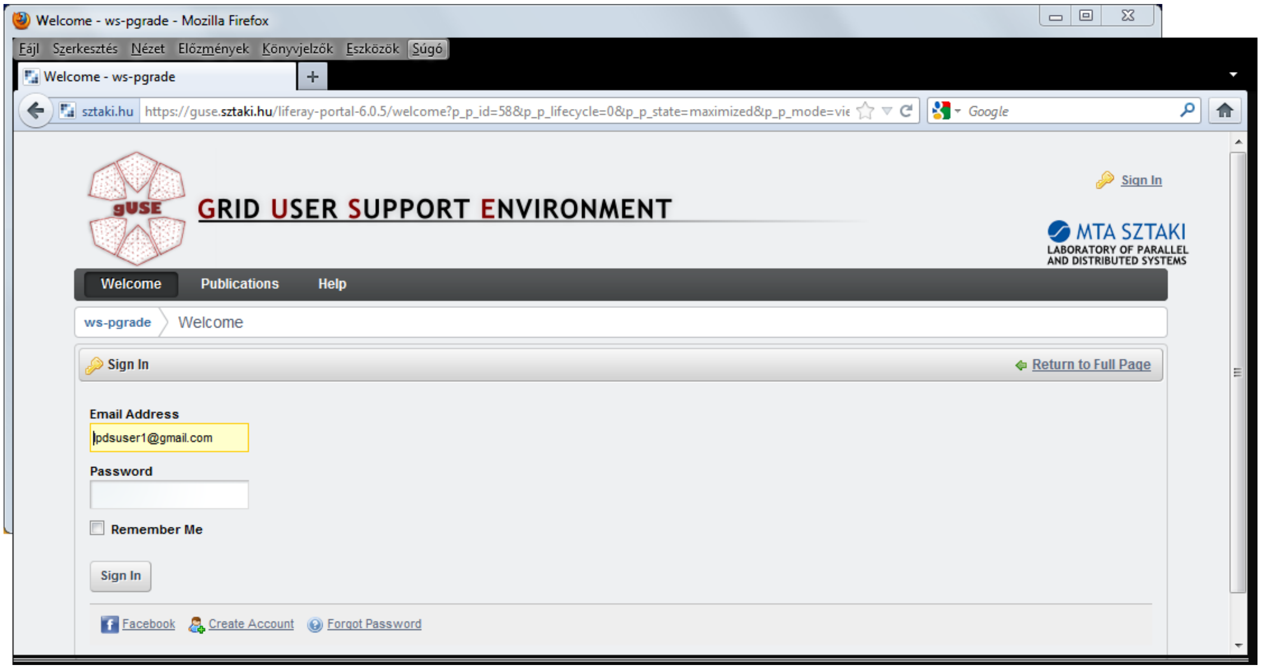

Welcome - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Welcome - ws-pgrade
sztaki.hu
https://guse.sztaki.hu/liferay-portal-6.0.5/
Google
Sign In
GRID USER SUPPORT ENVIRONMENT
MTA SZTAI
LABORATORY OF PARAL
AND DISTRIBUTED SYSTE
Welcome
Publications
Help
ws-pgrade
Welcome
Graphical User Interface: WS-PGRADE
Presentation tier
Workflow Storage
File Storage
Workflow Interpreter

Welcome to WS-PGRADE Portal!

The WS-PGRADE Portal, developed by Laboratory of Parallel and Distributed Systems at MTA-SZTAKI, Hungary is a web portal of the gUSE, grid User Support Environment. It supports development and submission of distributed applications executed on the computational

Figure 12.1

1.2 Select by click the upper right link *Sign In*:


Welcome - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Welcome - ws-pgrade
sztaki.hu
https://guse.sztaki.hu/liferay-portal-6.0.5/welcome?p_p_id=58&p_p_lifecycle=0&p_p_state=maximized&p_p_mode=vie
Google
Sign In
GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Publications
Help
ws-pgrade
Welcome
Sign In
Return to Full Page
Sign In
Facebook
Create Account
Forgot Password

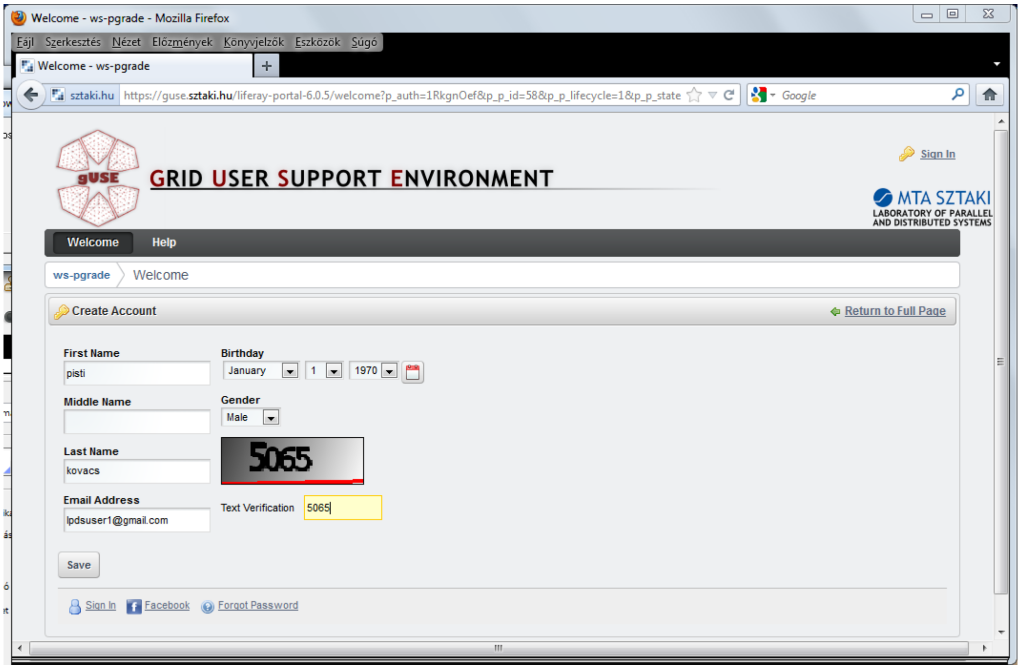
Email Address: pdsuser1@gmail.com

Password:

☐ Remember Me

Figure 12.2

1.3 Select by click the link *Create Account* toward the lower left corner:


Welcome - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Welcome - ws-pgrade
sztaki.hu https://guse.sztaki.hu/liferay-portal-6.0.5/welcome?p_auth=1RkgnOef&p_p_id=58&p_p_lifecycle=1&p_p_state
Google
gUSE
GRID USER SUPPORT ENVIRONMENT
Sign In
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Help
ws-pgrade
Welcome
Create Account
Return to Full Page
Save
Sign In
Facebook
Forgot Password

First Name: pisti

Middle Name:

Last Name: kovacs

Email Address: lpdsuser1@gmail.com

Birthday: January 1 1970

Gender: Male

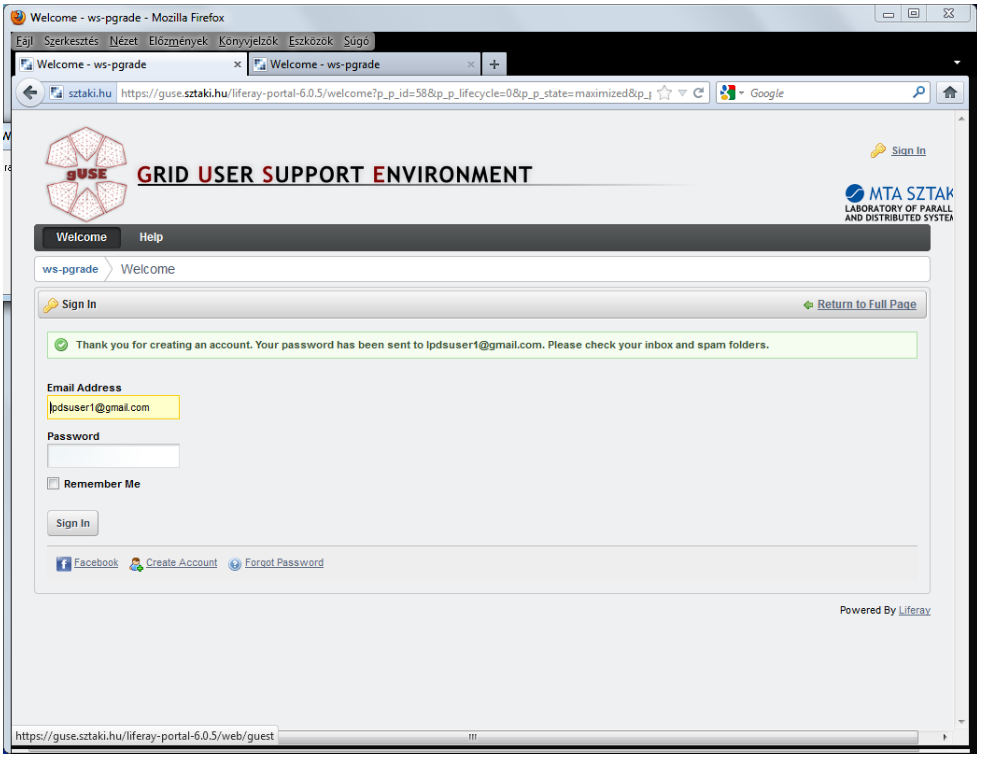
5065

Text Verification: 5065

Figure 12.3

Close the form by clicking on *Save* command.

1.4 You will get the answer similar to Figure 12.4:


Welcome - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Welcome - ws-pgrade
Welcome - ws-pgrade
sztaki.hu https://guse.sztaki.hu/liferay-portal-6.0.5/welcome?p_p_id=58&p_p_lifecycle=0&p_p_state=maximized&p_
Google
gUSE
GRID USER SUPPORT ENVIRONMENT
Sign In
MTA SZTAK
LABORATORY OF PARALL AND DISTRIBUTED SYSTEM
Welcome
Help
ws-pgrade
Welcome
Sign In
Return to Full Page
Sign In
Facebook
Create Account
Forgot Password
Powered By Liferay
https://guse.sztaki.hu/liferay-portal-6.0.5/web/guest

Thank you for creating an account. Your password has been sent to lpdsuser1@gmail.com. Please check your inbox and spam folders.

Email Address: lpdsuser1@gmail.com

Password:

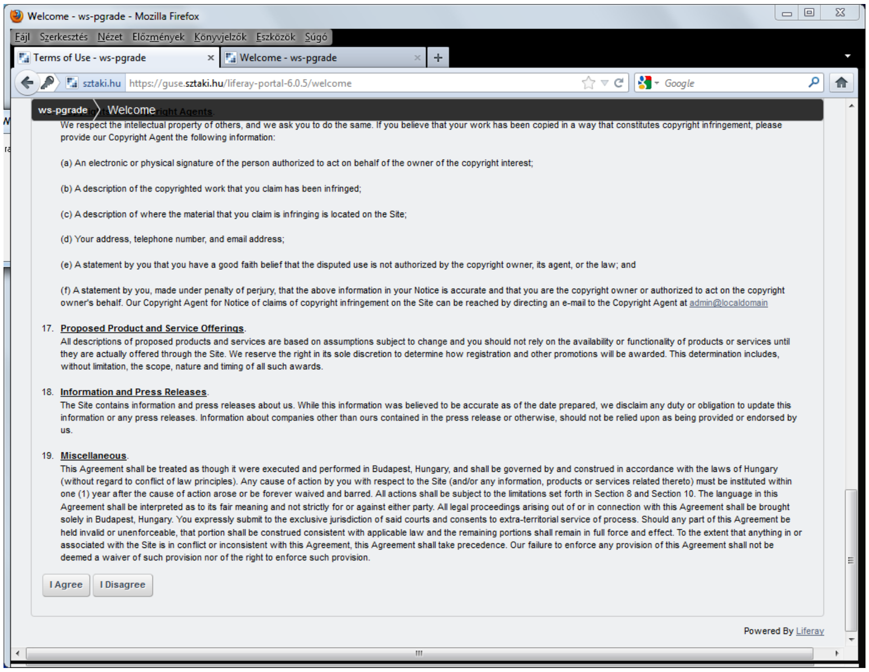
☐ Remember Me

Figure 12.4

You have to check your mail box, enter the generated password received there, and click on *Sign In*.

Note: this password can be changed later.

1.5 Accept terms of usage: You have received a restricted right to enter the portal. First you have to accept the term of usage:


Welcome - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Terms of Use - ws-pgrade
Welcome - ws-pgrade
sztaki.hu
https://guse.sztaki.hu/liferay-portal-6.0.5/welcome
Google
ws-pgrade
Welcome

We respect the intellectual property of others, and we ask you to do the same. If you believe that your work has been copied in a way that constitutes copyright infringement, please provide our Copyright Agent the following information:

(a) An electronic or physical signature of the person authorized to act on behalf of the owner of the copyright interest;

(b) A description of the copyrighted work that you claim has been infringed;

(c) A description of where the material that you claim is infringing is located on the Site;

(d) Your address, telephone number, and email address;

(e) A statement by you that you have a good faith belief that the disputed use is not authorized by the copyright owner, its agent, or the law; and

(f) A statement by you, made under penalty of perjury, that the above information in your Notice is accurate and that you are the copyright owner or authorized to act on the copyright owner's behalf. Our Copyright Agent for Notice of claims of copyright infringement on the Site can be reached by directing an e-mail to the Copyright Agent at admin@localdomain

17. **Proposed Product and Service Offerings**.
All descriptions of proposed products and services are based on assumptions subject to change and you should not rely on the availability or functionality of products or services until they are actually offered through the Site. We reserve the right in its sole discretion to determine how registration and other promotions will be awarded. This determination includes, without limitation, the scope, nature and timing of all such awards.

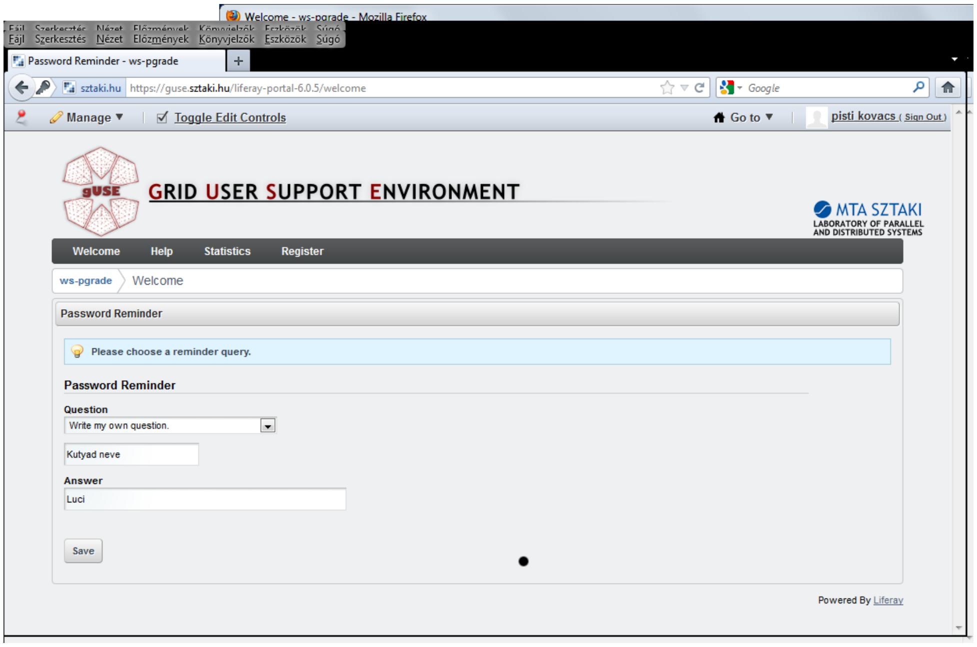
18. **Information and Press Releases**.
The Site contains information and press releases about us. While this information was believed to be accurate as of the date prepared, we disclaim any duty or obligation to update this information or any press releases. Information about companies other than ours contained in the press release or otherwise, should not be relied upon as being provided or endorsed by us.

19. **Miscellaneous**.
This Agreement shall be treated as though it were executed and performed in Budapest, Hungary, and shall be governed by and construed in accordance with the laws of Hungary (without regard to conflict of law principles). Any cause of action by you with respect to the Site (and/or any information, products or services related thereto) must be instituted within one (1) year after the cause of action arose or be forever waived and barred. All actions shall be subject to the limitations set forth in Section 8 and Section 10. The language in this Agreement shall be interpreted as to its fair meaning and not strictly for or against either party. All legal proceedings arising out of or in connection with this Agreement shall be brought solely in Budapest, Hungary. You expressly submit to the exclusive jurisdiction of said courts and consents to extra-territorial service of process. Should any part of this Agreement be held invalid or unenforceable, that portion shall be construed consistent with applicable law and the remaining portions shall remain in full force and effect. To the extent that anything in or associated with the Site is in conflict or inconsistent with this Agreement, this Agreement shall take precedence. Our failure to enforce any provision of this Agreement shall not be deemed a waiver of such provision nor of the right to enforce such provision.

I Agree
I Disagree
Powered By Liferay

Figure 12.5

1.6 The portal prompts you to define a password reminder:


Welcome - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Password Reminder - ws-pgrade
sztaki.hu
https://guse.sztaki.hu/liferay-portal-6.0.5/welcome
Google
Manage
Toggle Edit Controls
Go to
pisti kovacs (Sign Out)
gUSE
GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Help
Statistics
Register
ws-pgrade
Welcome
Password Reminder

Please choose a reminder query.

Password Reminder

Question: Write my own question.

Kutyad neve

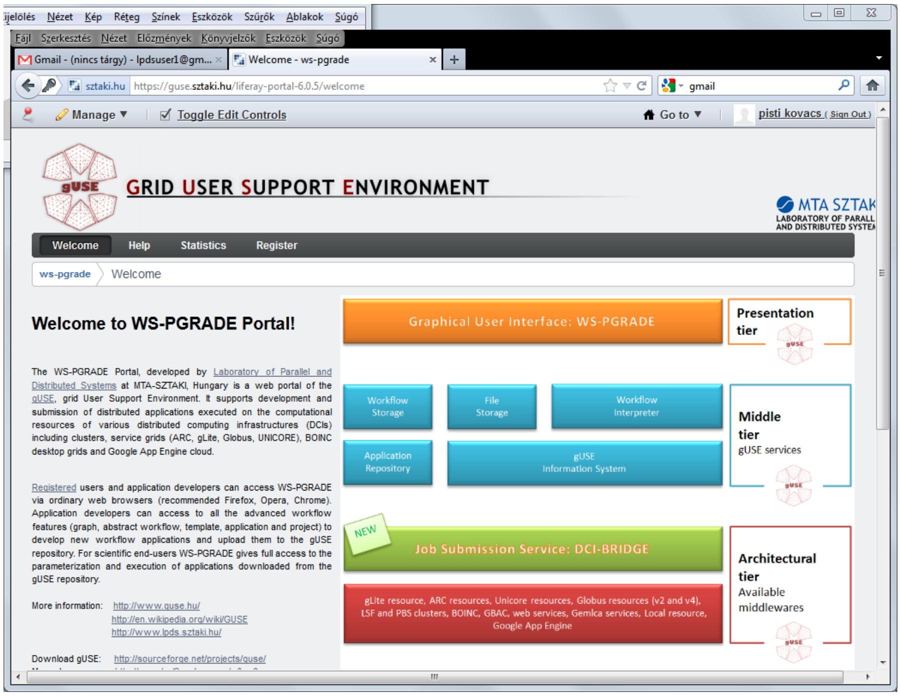
Answer: Luci

Save
Powered By Liferay

Figure 12.6

The user has to hit on *Save* button.

1.7 The next activity must be initiated by the user selecting the *Register* tab:


GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
Welcome
Help
Statistics
Register
ws-pgrade
Welcome
Graphical User Interface: WS-PGRADE
Presentation tier
Workflow Storage
File Storage
Workflow Interpreter
Application Repository
gUSE Information System
Middle tier
gUSE services
NEW
Job Submission Service: DCI-BRIDGE
gLite resource, ARC resources, Unicore resources, Globus resources (v2 and v4), LSF and PBS clusters, BOINC, GBAC, web services, Gemlca services, Local resource, Google App Engine
Architectural tier
Available middlewares

Welcome to WS-PGRADE Portal!

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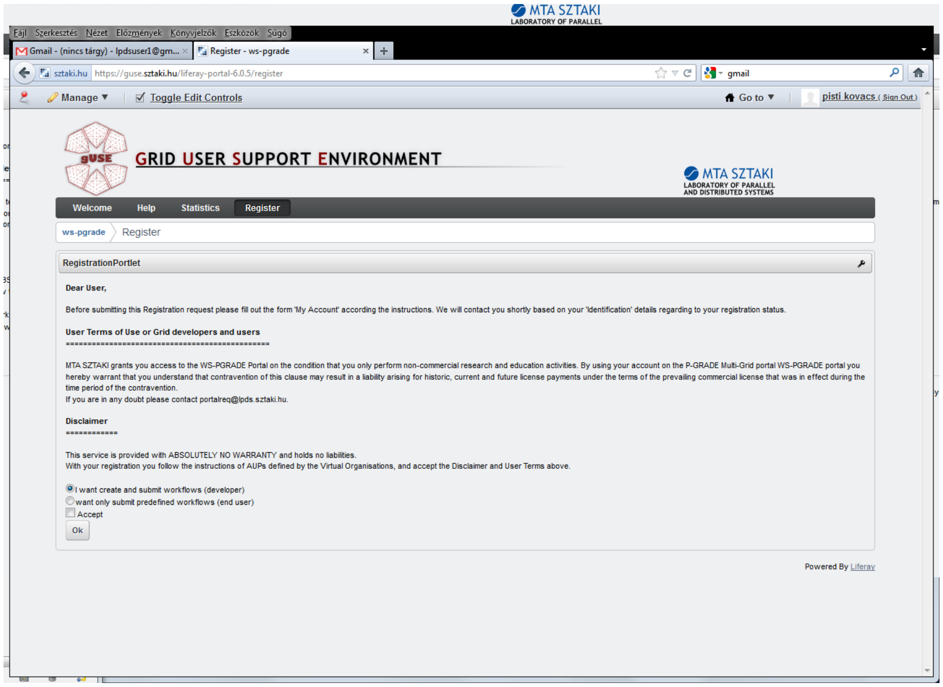
Registered users and application developers can access WS-PGRADE via ordinary web browsers (recommended Firefox, Opera, Chrome). Application developers can access to all the advanced workflow features (graph, abstract workflow, template, application and project) to develop new workflow applications and upload them to the gUSE repository. For scientific end-users WS-PGRADE gives full access to the parameterization and execution of applications downloaded from the gUSE repository.

More information: http://www.guse.hu/
http://en.wikipedia.org/wiki/GUSE
http://www.lpds.sztaki.hu/

Download gUSE: http://sourceforge.net/projects/guse/

Figure 12.7

1.8: Usage mode selection: The user can select between the developer and end-user regime within the *Register* tab (Figure 12.8).


GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Help
Statistics
Register
ws-pgrade
Register
RegistrationPortlet

Dear User,

Before submitting this Registration request please fill out the form 'My Account' according the instructions. We will contact you shortly based on your 'Identification' details regarding to your registration status.

User Terms of Use or Grid developers and users
==

MTA SZTAKI grants you access to the WS-PGRADE Portal on the condition that you only perform non-commercial research and education activities. By using your account on the P-GRADE Multi-Grid portal WS-PGRADE portal you hereby warrant that you understand that contravention of this clause may result in a liability arising for historic, current and future license payments under the terms of the prevailing commercial license that was in effect during the time period of the contravention.
If you are in any doubt please contact portalreq@lpds.sztaki.hu.

Disclaimer
============

This service is provided with ABSOLUTELY NO WARRANTY and holds no liabilities.
With your registration you follow the instructions of AUPs defined by the Virtual Organisations, and accept the Disclaimer and User Terms above.

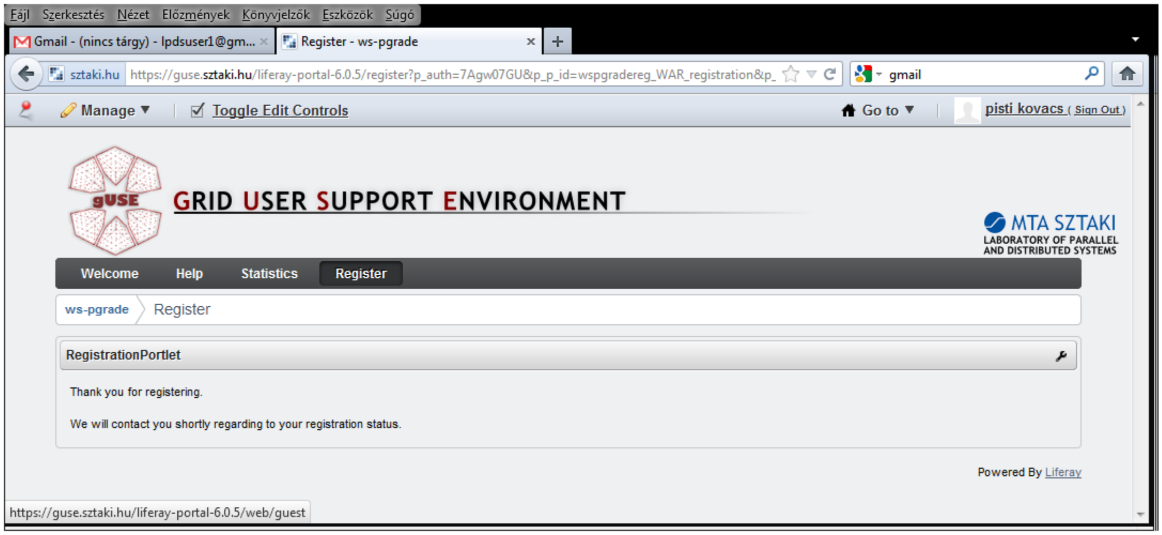
● I want create and submit workflows (developer)
○ want only submit predefined workflows (end user)
☐ Accept
Ok

Powered By Liferay

Figure 12.8

Do not forget to set the *Accept* check box before closing this step by the *OK* button.

1.9: The user receives a message from the system that the account request has been forwarded to arbitration:

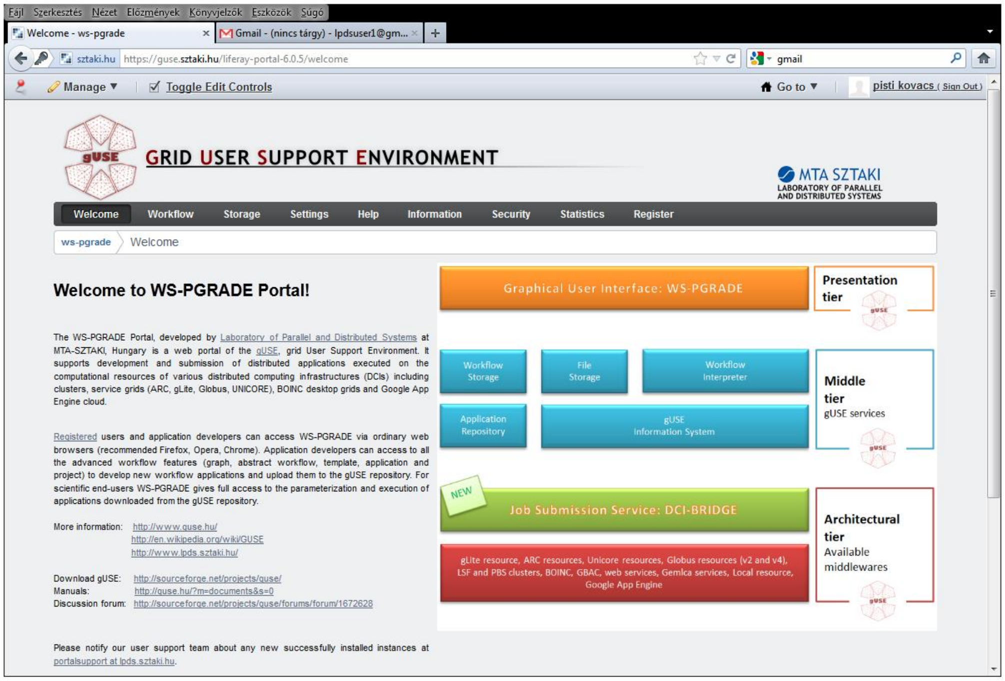

Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Gmail - (nincs tárgy) - lpdsuser1@gm...
Register - ws-pgrade
sztaki.hu https://guse.sztaki.hu/liferay-portal-6.0.5/register?p_auth=7Agw07GU&p_p_id=wspgradereg_WAR_registration&p_
gmail
Manage ▼
Toggle Edit Controls
Go to ▼
pisti kovacs (Sign Out)
GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Help
Statistics
Register
ws-pgrade
Register
RegistrationPortlet
Powered By Liferay
https://guse.sztaki.hu/liferay-portal-6.0.5/web/guest

Thank you for registering.

We will contact you shortly regarding to your registration status.

Figure 12.9

1.10: Finally, receiving the confirming e-mail and signing in the portal once again (see Figure 12.2), the user will see all the functionalities need to be able playing in the selected role:


Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Welcome - ws-pgrade
Gmail - (nincs tárgy) - lpdsuser1@gm...
sztaki.hu https://guse.sztaki.hu/liferay-portal-6.0.5/welcome
gmail
Manage ▼
Toggle Edit Controls
Go to ▼
pisti kovacs (Sign Out)
GRID USER SUPPORT ENVIRONMENT
MTA SZTAKI
LABORATORY OF PARALLEL AND DISTRIBUTED SYSTEMS
Welcome
Workflow
Storage
Settings
Help
Information
Security
Statistics
Register
ws-pgrade
Welcome
Graphical User Interface: WS-PGRADE
Presentation tier
Workflow Storage
File Storage
Workflow Interpreter
Application Repository
gUSE Information System
Middle tier
gUSE services
NEW
Job Submission Service: DCI-BRIDGE
gLite resource, ARC resources, Unicore resources, Globus resources (v2 and v4), LSF and PBS clusters, BOINC, GBAC, web services, Gemlca services, Local resource, Google App Engine
Architectural tier
Available middlewares

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More information:	http://www.guse.hu/ http://en.wikipedia.org/wiki/GUSE http://www.lpds.sztaki.hu/
Download gUSE:	http://sourceforge.net/projects/guse/
Manuals:	http://guse.hu/?m=documents&s=0
Discussion forum:	http://sourceforge.net/projects/guse/forums/forum/1672628

Please notify our user support team about any new successfully installed instances at portalsupport at lpds.sztaki.hu.

Figure 12.10

2. Change password

2.1 Select the *Manage* menu in upper left corner of the portal:

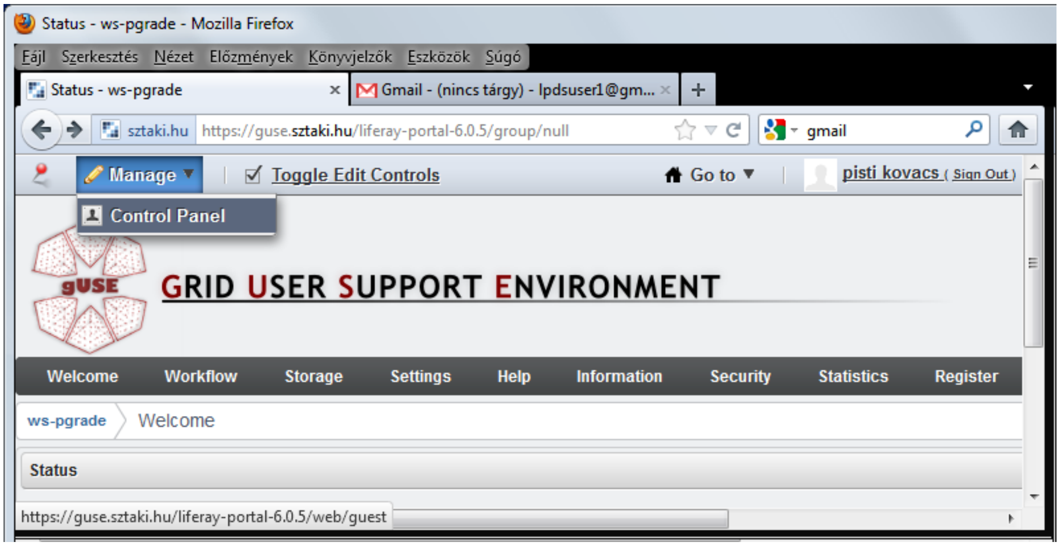
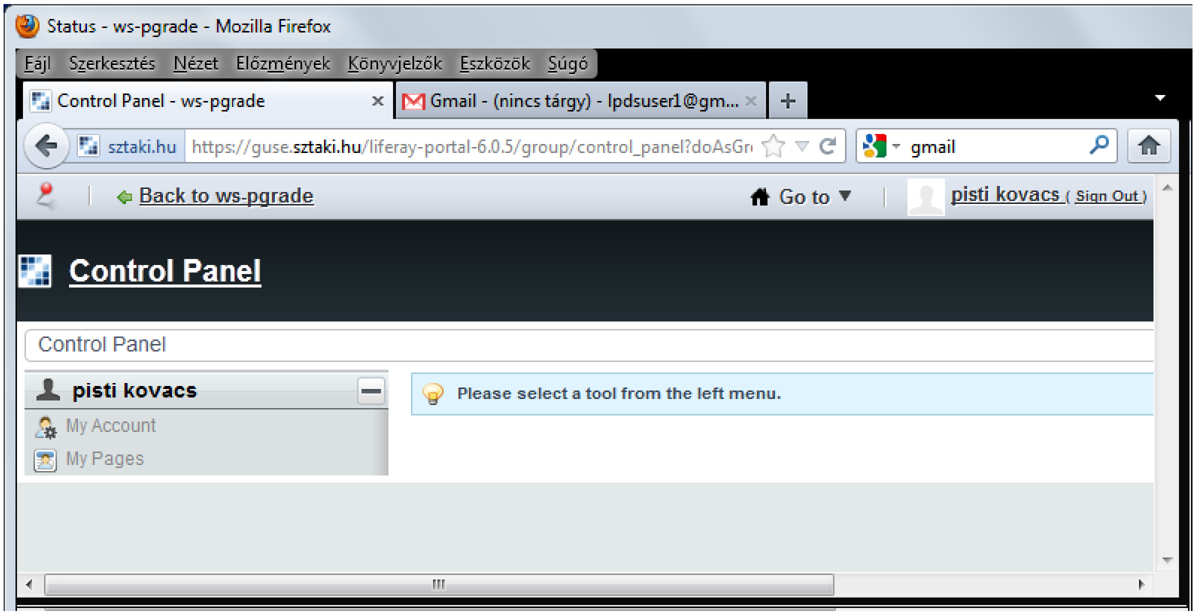

Status - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Status - ws-pgrade
Gmail - (nincs tárgy) - lpdsuser1@gm...
sztaki.hu https://guse.sztaki.hu/liferay-portal-6.0.5/group/null
gmail
Manage
Toggle Edit Controls
Go to
pisti kovacs (Sign Out)
Control Panel
GRID USER SUPPORT ENVIRONMENT
Welcome
Workflow
Storage
Settings
Help
Information
Security
Statistics
Register
ws-pgrade
Welcome
Status
https://guse.sztaki.hu/liferay-portal-6.0.5/web/guest

Figure 12.11

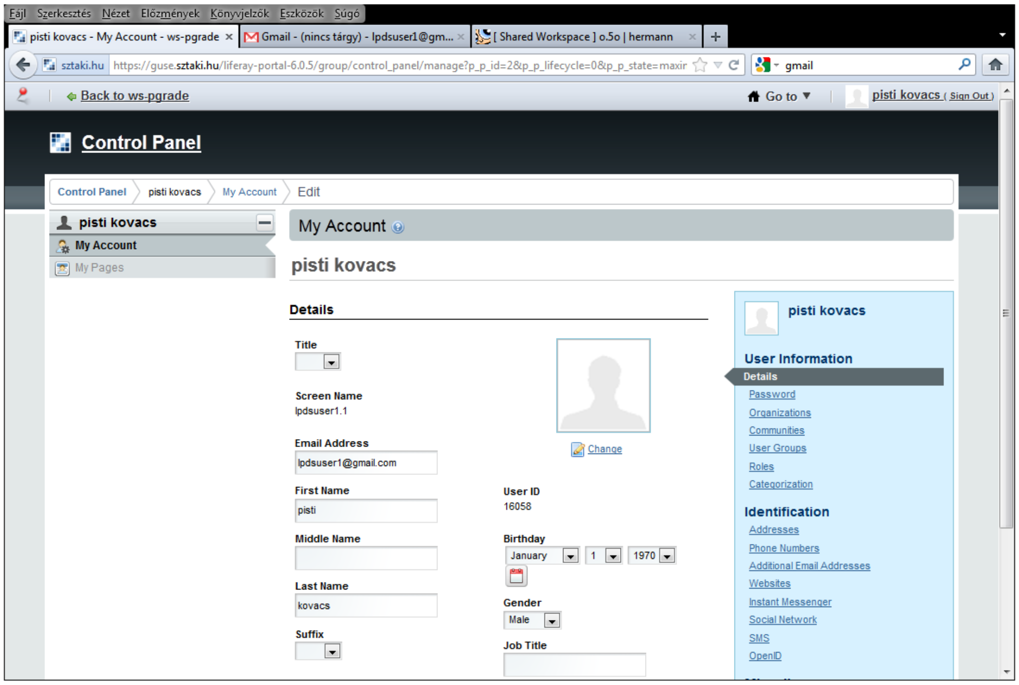
2.2 Choose the *Control Panel* menu item:


Status - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
Control Panel - ws-pgrade
Gmail - (nincs tárgy) - lpdsuser1@gm...
sztaki.hu https://guse.sztaki.hu/liferay-portal-6.0.5/group/control_panel?doAsGr
gmail
Back to ws-pgrade
Go to
pisti kovacs (Sign Out)
Control Panel
Control Panel
pisti kovacs
My Account
My Pages

Please select a tool from the left menu.

Figure 12.12

Choose the *My Account* menu item of the header showing the name of the user ("pisti kovacs" on Figure 12.13):


Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
pisti kovacs - My Account - ws-pgrade
Gmail - (nincs tárgy) - lpdsuser1@gm...
[Shared Workspace] o.5o | hermann
https://guse.sztaki.hu/liferay-portal-6.0.5/group/control_panel/manage?p_p_id=2&p_p_lifecycle=0&p_p_state=maxir
gmail
Back to ws-pgrade
Go to
pisti kovacs (Sign Out)
Control Panel
Control Panel
pisti kovacs
My Account
Edit
pisti kovacs
My Account
My Pages
My Account
pisti kovacs
Details
Change
pisti kovacs
User Information
Details
Password
Organizations
Communities
User Groups
Roles
Categorization
Identification
Addresses
Phone Numbers
Additional Email Addresses
Websites
Instant Messenger
Social Network
SMS
OpenID

Title:

Screen Name: lpdsuser1.1

Email Address: lpdsuser1@gmail.com

First Name: pisti

Middle Name:

Last Name: kovacs

Suffix:

User ID: 16058

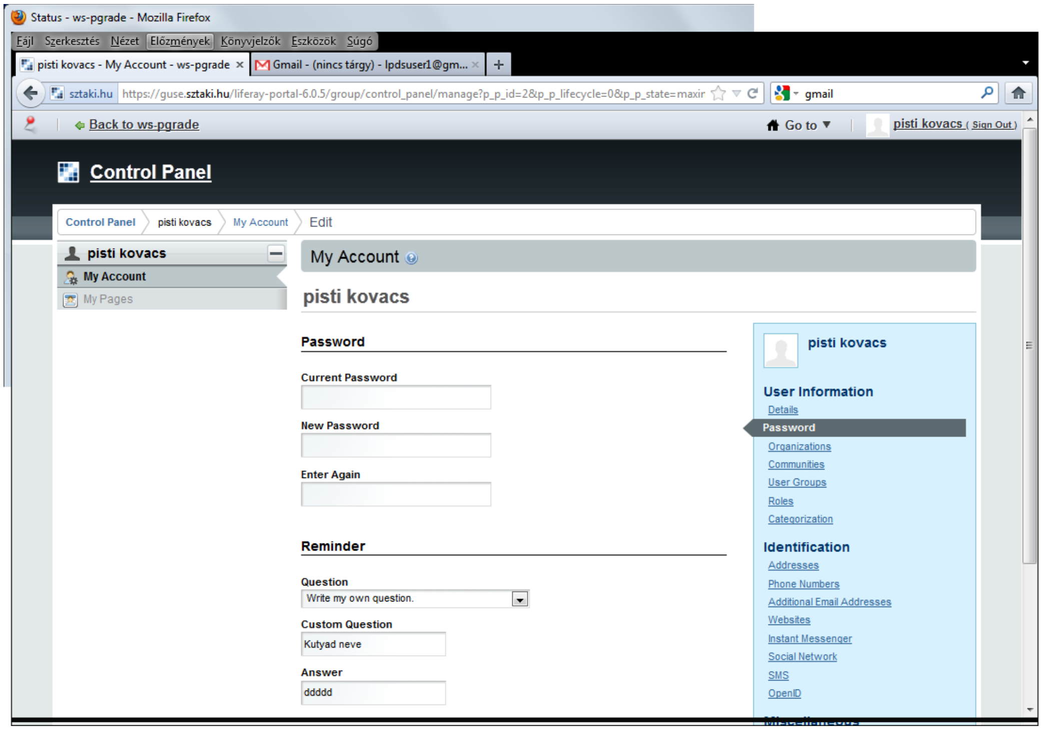
Birthday: January 1 1970

Gender: Male

Job Title:

Figure 12.13

Select the *Password* link from the right hand side *User Information* table (see Figure 12.14):


Status - ws-pgrade - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
pisti kovacs - My Account - ws-pgrade
Gmail - (nincs tárgy) - lpdsuser1@gm...
https://guse.sztaki.hu/liferay-portal-6.0.5/group/control_panel/manage?p_p_id=2&p_p_lifecycle=0&p_p_state=maxir
gmail
Back to ws-pgrade
Go to
pisti kovacs (Sign Out)
Control Panel
Control Panel
pisti kovacs
My Account
Edit
pisti kovacs
My Account
My Pages
My Account
pisti kovacs
Password
Reminder
pisti kovacs
User Information
Details
Password
Organizations
Communities
User Groups
Roles
Categorization
Identification
Addresses
Phone Numbers
Additional Email Addresses
Websites
Instant Messenger
Social Network
SMS
OpenID
Miscellaneous

Current Password:

New Password:

Enter Again:

Question: Write my own question.

Custom Question: Kutyad neve

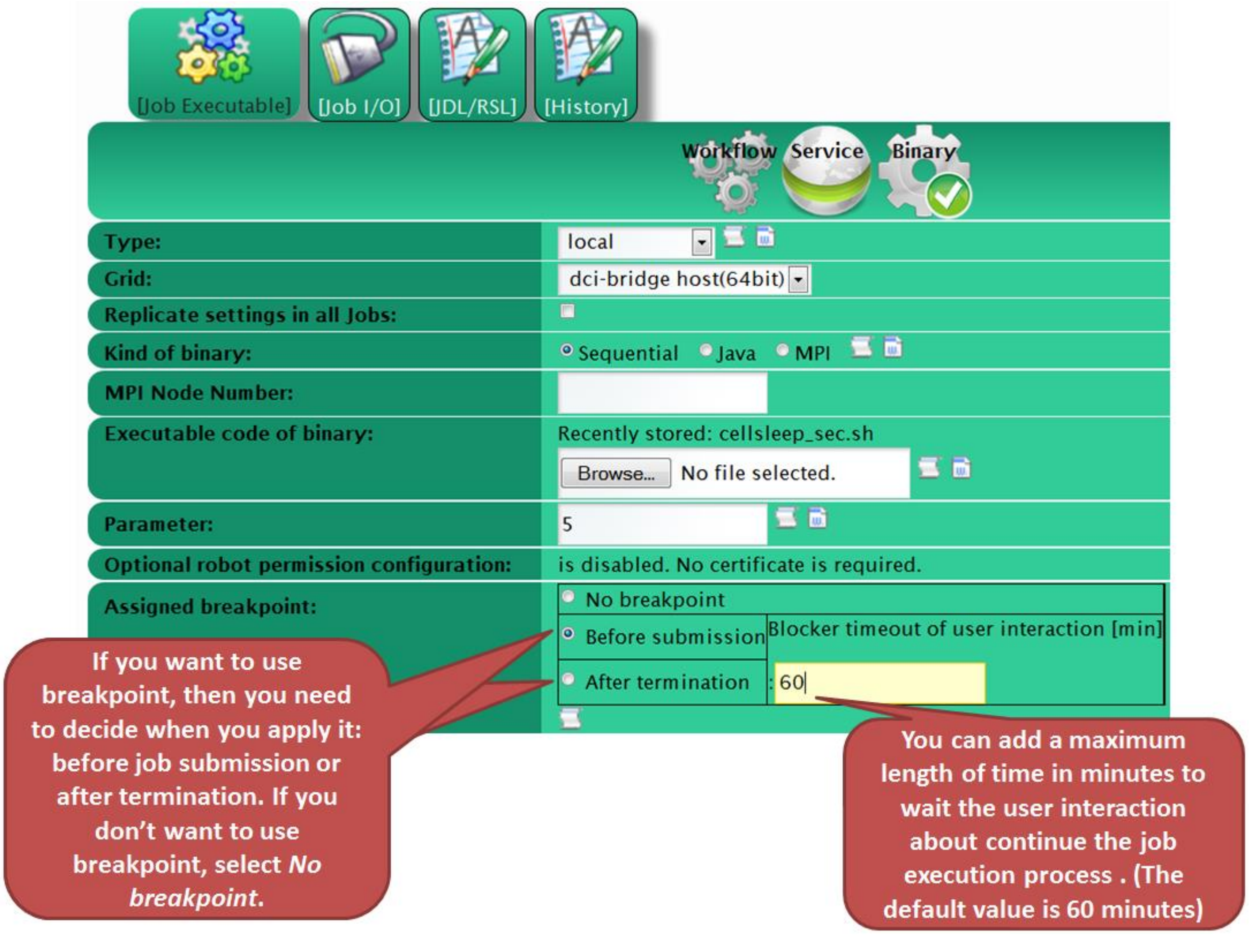
Answer: ddddd

Figure 12.14

Note: Do not forget *Save* the form after the proper filling the fields *Current Password*, *New Password* and *Enter Again*.

13. Debugging of Job Submissions by Breakpoints

The user can define job associated breakpoints during workflow configuration in order to control the runtime execution of the created job instances. All instances of a job marked by a breakpoint will contain this breakpoint in the job submission process. The workflow interpreter detects the defined breakpoints during the elaboration of the job instances and notifies the user about the temporary suspension of the job instance associated activity by proper job state changing. The user polling the states of job instances may decide separately about the future of each suspended job instance related activity by enabling or prohibiting its progress. Moreover, the user may change the configuration of the workflow after a global *Suspend* command issued in a "break pointed" state.



Type:	local
Grid:	dci-bridge host(64bit)
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	Recently stored: cellsleep_sec.sh Browse... No file selected.
Parameter:	5
Optional robot permission configuration:	is disabled. No certificate is required.
Assigned breakpoint:	○ No breakpoint ● Before submission ○ After termination Blocker timeout of user interaction [min]: 60

If you want to use breakpoint, then you need to decide when you apply it: before job submission or after termination. If you don't want to use breakpoint, select *No breakpoint*.

You can add a maximum length of time in minutes to wait the user interaction about continue the job execution process . (The default value is 60 minutes)

Figure 13.1 Breakpoint setting of a job in the WS-PGRADE *Configure* function within the *Job Executable* tab

Breakpoint definition as a part of the Job Configuration

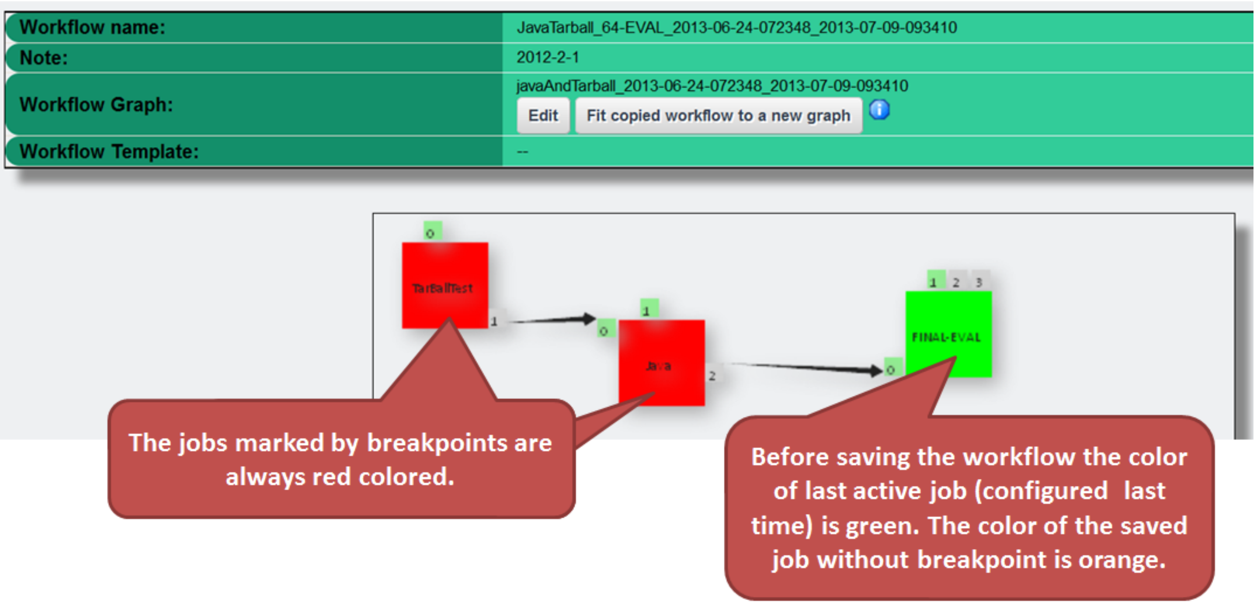
The breakpoint settings (see Fig. 13.1) are the part of a job configuration in the *Job Executable* tab within *Configure* function. On one hand you have to decide whether or not you assign a breakpoint to the given job. On the other hand you can define the role of the breakpoint choosing from the two real options:

- You can assign breakpoint *before* the *submission* of a job (in this case you can check and modify the running of the associated subsequent job instances of the workflow directly before starting them) or
- *after job termination* (in this case the associated job instances are submitted and executed, and the user can interact after the termination of the associated job instances. Therefore the user has all additional information can be gained from the results of the executed job instances.)

Additionally, the user must set an expiration time: the maximum time length for waiting the user interaction after breakpoint detection. This value is defined in minutes in both (before and after) cases. (The default value is 60 minutes.). Reaching the defined breakpoint and after expiration the system will not wait any longer for the user intervention and the associated job instance will be either aborted (in case of "Before submission" kind breakpoints) or its output will not be forwarded toward other jobs (in case of "After termination" kind breakpoints)

The value must be a natural number. The workflow interpreter polls the expiration condition with a 1 minute sampling frequency.

The workflow configuration graph discriminates the jobs associated with active breakpoint settings by red color (see Fig. 13.2.).



Workflow name:	JavaTarball_64-EVAL_2013-06-24-072348_2013-07-09-093410
Note:	2012-2-1
Workflow Graph:	javaAndTarball_2013-06-24-072348_2013-07-09-093410
Workflow Template:	--

The jobs marked by breakpoints are always red colored.

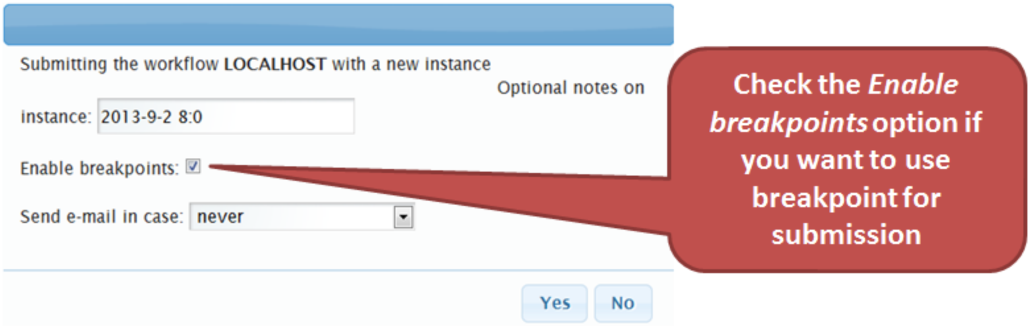
Before saving the workflow the color of last active job (configured last time) is green. The color of the saved job without breakpoint is orange.

Figure 13.2 The view of a workflow containing jobs configured with breakpoints

You can apply breakpoint settings at the workflow templates, too. You can create templates from workflows configured with breakpoints and you can use templates derived from this workflows.

Workflow submission in debugging state

Once you have configured and saved your workflow, you can submit it by clicking on *Submit* button in the *Concrete* window. In the pop-up dialog box you can check the *Enable breakpoints* option to enable the debugging of your workflow during submission (Fig. 13.3). If you choose this option but your workflow application (neither the main nor the eventual embedded workflows) contain no breakpoint association then you will get back the configuration window of the workflow (Fig. 13.1) to configure breakpoint directly after clicking on *Yes*.



Submitting the workflow **LOCALHOST** with a new instance

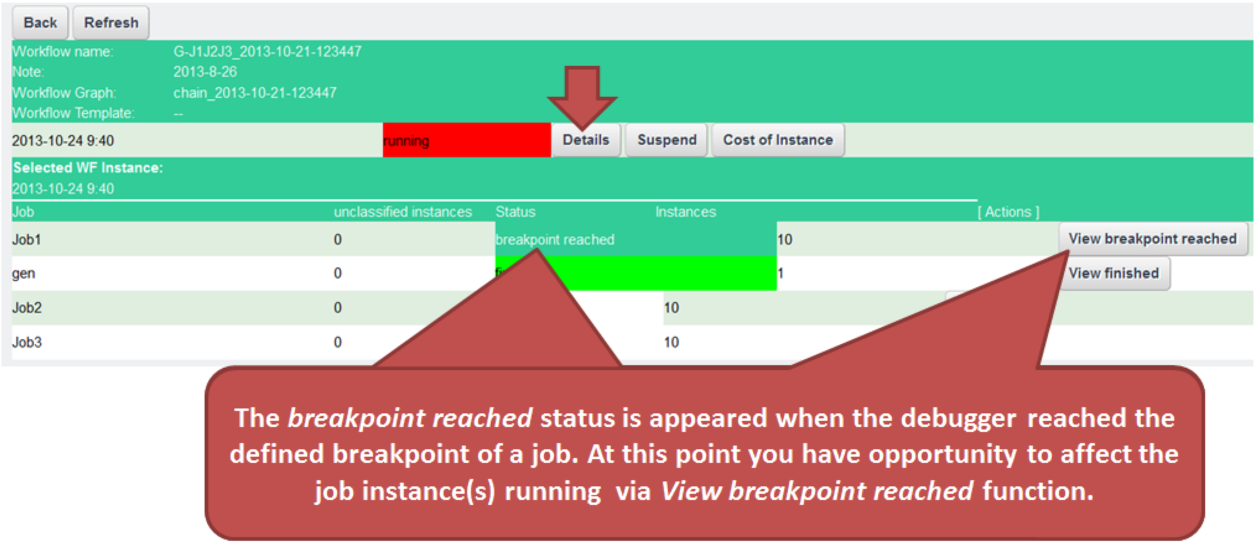
Optional notes on instance: 2013-9-2 8:0

Enable breakpoints: ☑

Send e-mail in case: never

Check the ***Enable breakpoints*** option if you want to use breakpoint for submission

Figure 13.3 The pop-up window at the startup of submission together with *Enable breakpoints* checkbox



Workflow name: G-J1J2J3_2013-10-21-123447
Note: 2013-8-26
Workflow Graph: chain_2013-10-21-123447
Workflow Template: --

2013-10-24 9:40 running

Selected WF Instance:
2013-10-24 9:40

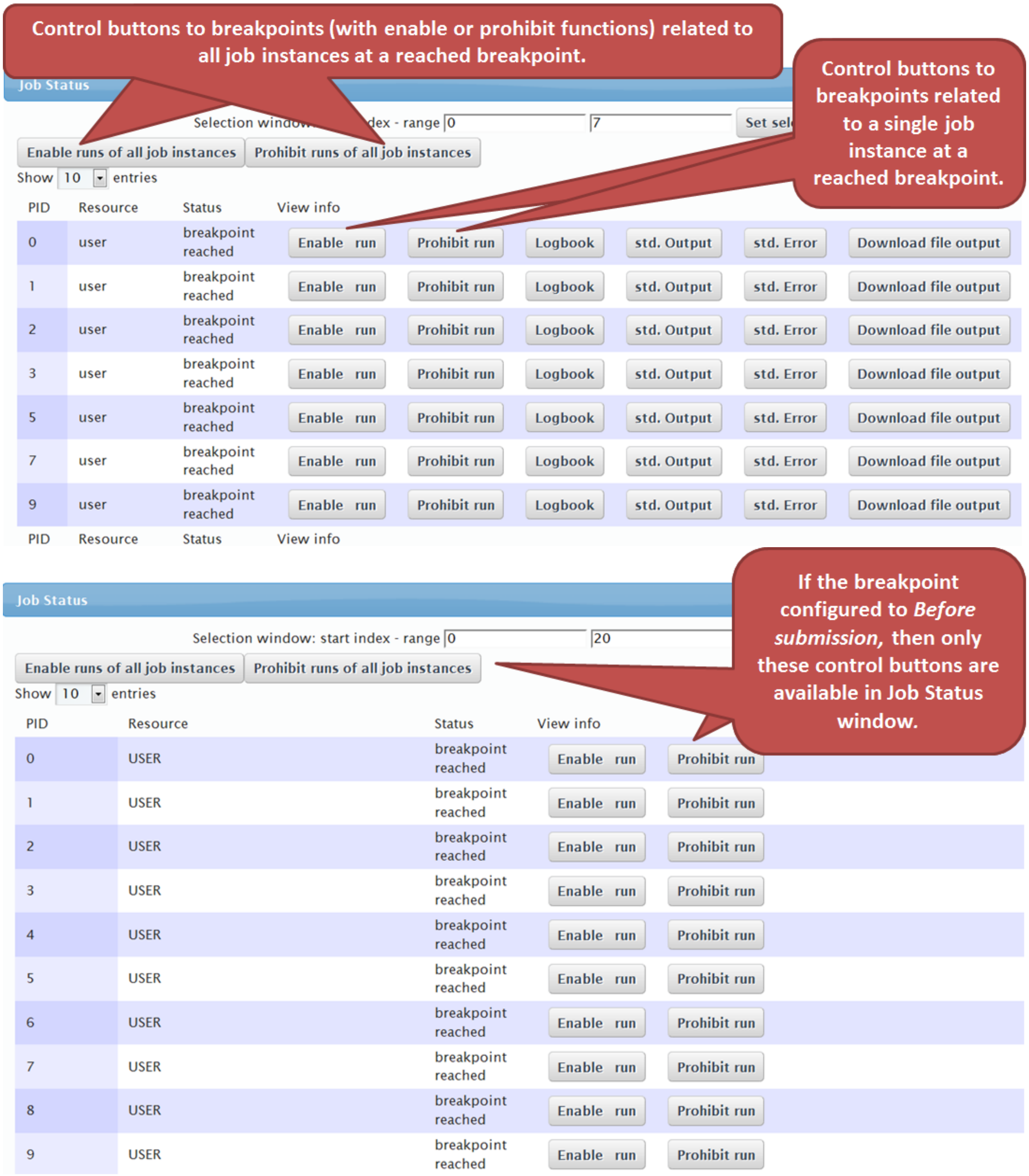
Job	unclassified instances	Status	Instances	[Actions]
Job1	0	breakpoint reached	10	View breakpoint reached
gen	0		1	View finished
Job2	0		10	
Job3	0		10	

The *breakpoint reached* status is appeared when the debugger reached the defined breakpoint of a job. At this point you have opportunity to affect the job instance(s) running via *View breakpoint reached* function.

Figure 13.4 *Breakpoint reached* status message within the *Details* function of running workflow instance

After you have started the workflow, you can trace the job instances of the workflow instance by clicking on the proper *Details* button in the *Workflow/Concrete* page. You may select the running workflow instance from the appearing list and by clicking of the corresponding *Details* button you get the job group map of the selected workflow instance. From this point, you can interact with the workflow instance in runtime at the defined breakpoints. The appearance of the sub group "breakpoint reached" indicates that at least one instance of the given job hangs up on a breakpoint (Fig. 13.4).

Pitfall: Very rarely, the system can't detect the actual status of a job instance. In this case, the column of *unclassified instances* in the *Concrete/Details* window shows the number of job instances being in this transient state (see Fig. 13.4). Please, use the *Refresh* button and wait a couple of moment until the value of *unclassified instances* changes to 0 again.



Control buttons to breakpoints (with enable or prohibit functions) related to all job instances at a reached breakpoint.

Control buttons to breakpoints related to a single job instance at a reached breakpoint.

Job Status

Selection window: start index - range 0 7

Set sel
Enable runs of all job instances
Prohibit runs of all job instances
Show 10 entries

PID	Resource	Status	View info
0	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
1	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
2	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
3	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
5	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
7	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
9	user	breakpoint reached	Enable run Prohibit run Logbook std. Output std. Error Download file output
PID	Resource	Status	View info

If the breakpoint configured to *Before submission*, then only these control buttons are available in Job Status window.

Job Status

Selection window: start index - range 0 20

Enable runs of all job instances
Prohibit runs of all job instances
Show 10 entries

PID	Resource	Status	View info
0	USER	breakpoint reached	Enable run Prohibit run
1	USER	breakpoint reached	Enable run Prohibit run
2	USER	breakpoint reached	Enable run Prohibit run
3	USER	breakpoint reached	Enable run Prohibit run
4	USER	breakpoint reached	Enable run Prohibit run
5	USER	breakpoint reached	Enable run Prohibit run
6	USER	breakpoint reached	Enable run Prohibit run
7	USER	breakpoint reached	Enable run Prohibit run
8	USER	breakpoint reached	Enable run Prohibit run
9	USER	breakpoint reached	Enable run Prohibit run

Figure 13.5 *Job Status* windows in case of a reached breakpoint that configured *After termination* (upper side) and *Before submission* (under side) of a job instance.

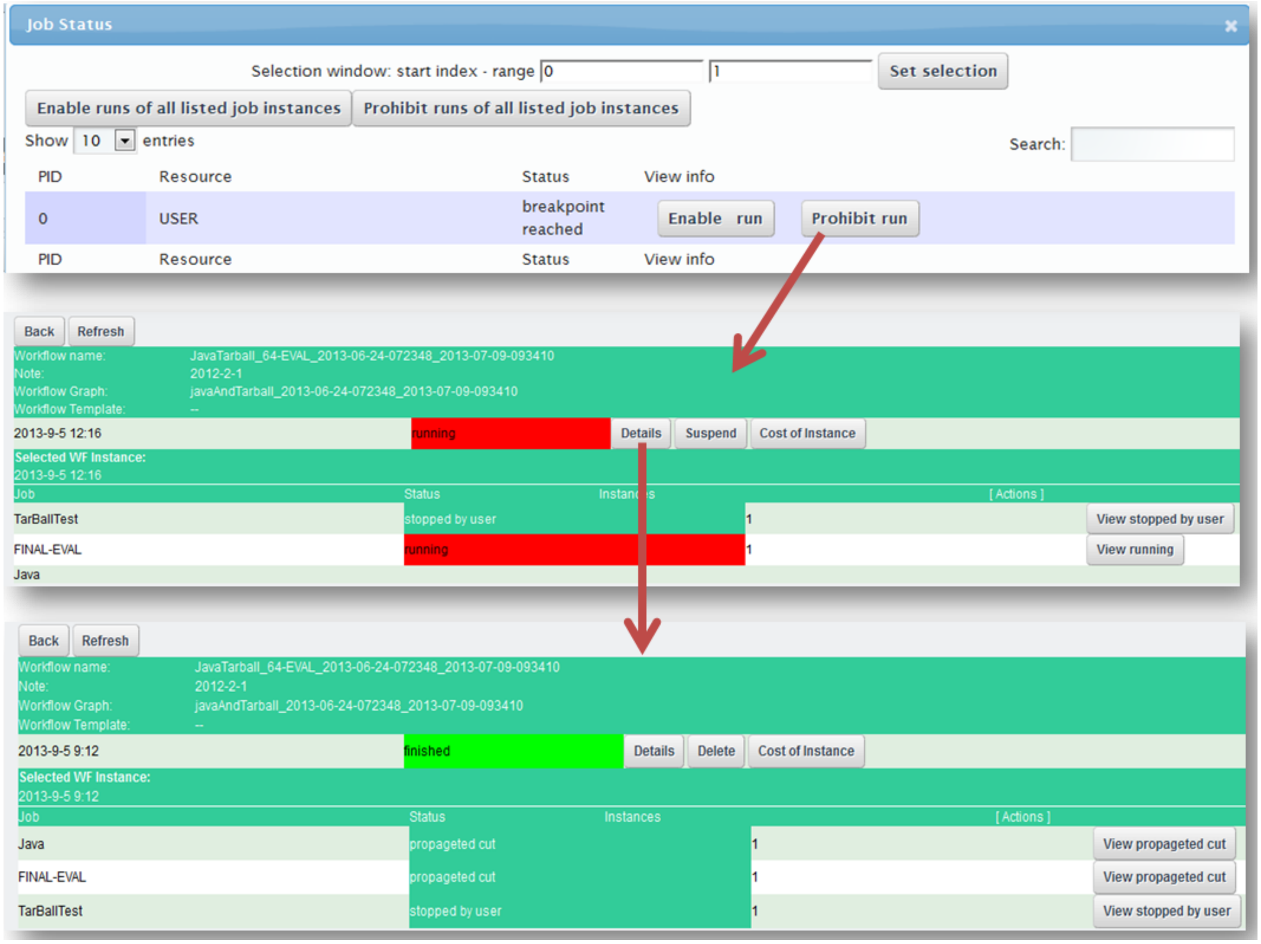
For debugging your workflow, use the *View breakpoint reached* button (Fig. 13.4). After clicking on it, you can choose from two available options: enable running of selected job instance (*Enable run*) or prohibit running (*Prohibit run*). If you want to enable or prohibit all job instances running at breakpoint, you don't need to click the buttons one after the other but you can click on *Enable runs of all job instances* button or on *Prohibit runs of all job instances* button depending on your decision.

Note: The issued commands *Enable runs of all job instances* and *Prohibit runs of all job instances* have effect not only on the job instances being hanging on the breakpoint but they determine the fate of the instances which will reach the defined breakpoint in the future as well.

If the breakpoint is configured as "*After termination",* then you may get additional information about the submission of a job instance by clicking on the already well-known info buttons (for details see chapter 3.1 within the *Menu-Oriented Online Help*): *Logbook, std. Output, std. Error,* and *Download file output*. Certainly, this info buttons are not available when the breakpoint is configured to *Before submission* (Fig. 13.5).

Note: Sometimes the user interface logs behind the reality and the *breakpoint reached* function of the user interface doesn't provide just-in-time information about the states of job instances: for a short time the intervention of the user seems to be not happened. This may occur in cases when a high number of job instances are hanging on a "*Before submission*" breakpoint, and when a collective command (*Enable runs of all job instances* or *Prohibit runs of all job instances*) is issued.

Depending on your decision, the job status will be changed. If you prohibit the further activity related a job instance by clicking on the *Prohibit run* button, then you will get the status "*stopped by user*" shown by Fig. 13.6 (You can refresh the status time after time by clicking on *Details* button. The effect of this termination operation will be propagated to the other job instances of workflow instance, the status of subsequent job instances will be "*propagated cut"* (Fig. 13.6). (It is important to emphasize again: a simple breakpoint operation (Enable run, Prohibit run) refers always to a single job instance, thus it is independent from other job instances of the same workflow.)


Job Status
Set selection
Enable runs of all listed job instances
Prohibit runs of all listed job instances
Show 10 entries
Search:
Enable run
Prohibit run
Back
Refresh
Details
Suspend
Delete
Cost of Instance

Selection window: start index - range 0 1

PID	Resource	Status	View info
0	USER	breakpoint reached	Enable run Prohibit run

Workflow name: JavaTarball_64-EVAL_2013-06-24-072348_2013-07-09-093410
Note: 2012-2-1
Workflow Graph: javaAndTarball_2013-06-24-072348_2013-07-09-093410
Workflow Template: --

2013-9-5 12:16 running

Selected WF Instance:
2013-9-5 12:16

Job	Status	Instances	[Actions]
TarBallTest	stopped by user	1	View stopped by user
FINAL-EVAL	running	1	View running
Java			

Workflow name: JavaTarball_64-EVAL_2013-06-24-072348_2013-07-09-093410
Note: 2012-2-1
Workflow Graph: javaAndTarball_2013-06-24-072348_2013-07-09-093410
Workflow Template: --

2013-9-5 9:12 finished

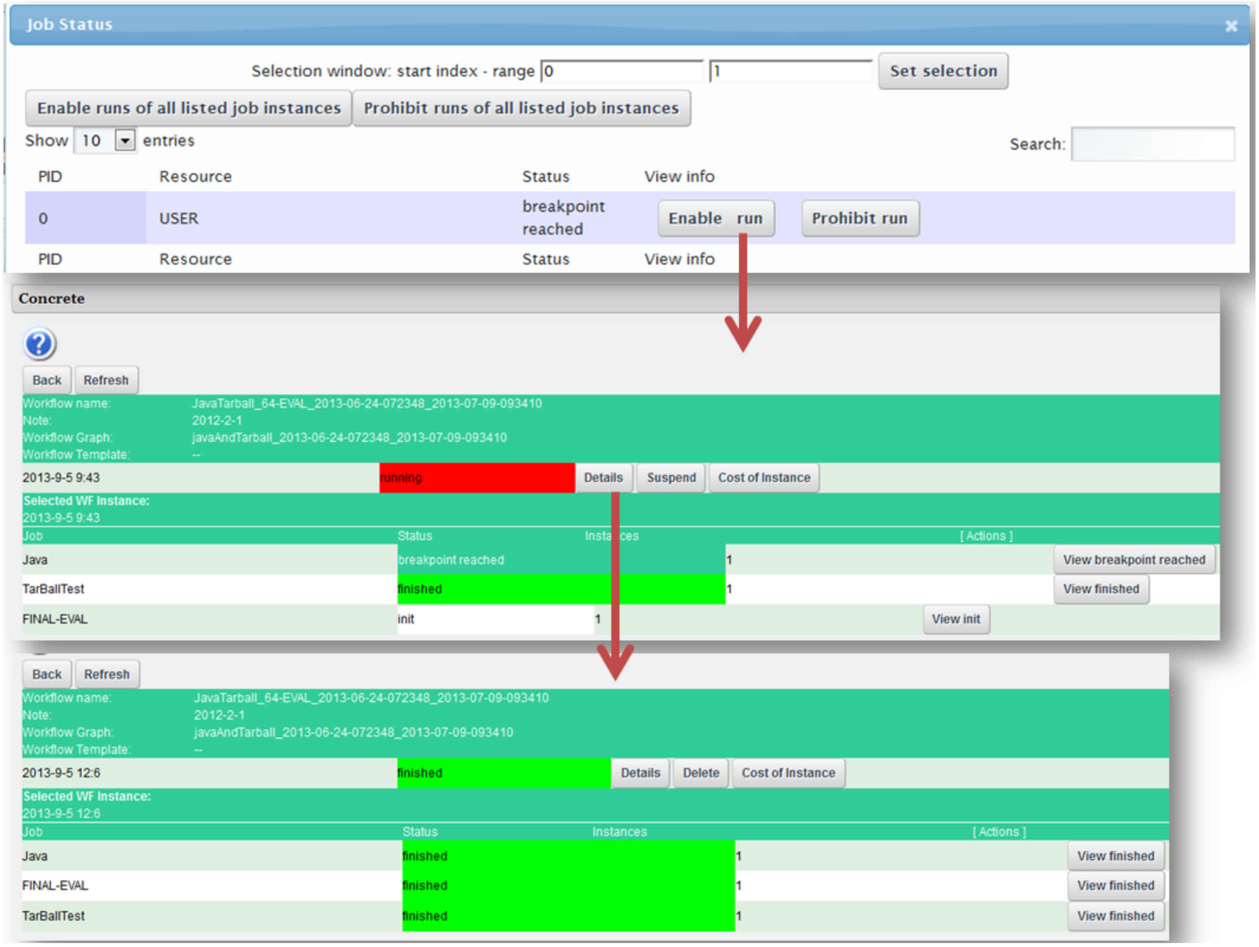
Selected WF Instance:
2013-9-5 9:12

Job	Status	Instances	[Actions]
Java	propagated cut	1	View propagated cut
FINAL-EVAL	propagated cut	1	View propagated cut
TarBallTest	stopped by user	1	View stopped by user

Figure 13.6 The effect of a prohibition of running a job instance.

The user intervention “Enable run” (see Fig. 13.7) terminates the suspension of the related job activity: the state of the job instance will be either “submitted” in case of the “before submission” kind of breakpoint or “finished”/”error” in case of the “after termination” kind one.

Note: Please remember that you have just a restricted time interval for making your selection between enabling or prohibiting the progress of the thread associated to the suspended job instance: a previously defined “Blocker timeout of user interaction” mentioned in job configuration section (see Fig. 13.1). Eventual expiration of this time stops the activity of the thread related to job instance hanging on this breakpoint (you get the *stopped due to timeout* status message) and then the whole workflow instance is aborted (see Fig. 13.8).


Job Status
Set selection
Enable runs of all listed job instances
Prohibit runs of all listed job instances
Show 10 entries
Search:
Enable run
Prohibit run
Concrete
Back
Refresh
Details
Suspend
Cost of Instance
View breakpoint reached
View finished
View init
Back
Refresh
Details
Delete
Cost of Instance
View finished
View finished
View finished

Selection window: start index - range 0 1

PID	Resource	Status	View info
0	USER	breakpoint reached	
PID	Resource	Status	View info

Workflow name: JavaTarball_64-EVAL_2013-06-24-072348_2013-07-09-093410
Note: 2012-2-1
Workflow Graph: javaAndTarball_2013-06-24-072348_2013-07-09-093410
Workflow Template: --

2013-9-5 9:43 running

Selected WF Instance:
2013-9-5 9:43

Job	Status	Instances	[Actions]
Java	breakpoint reached	1	View breakpoint reached
TarBallTest	finished	1	View finished
FINAL-EVAL	init	1	View init

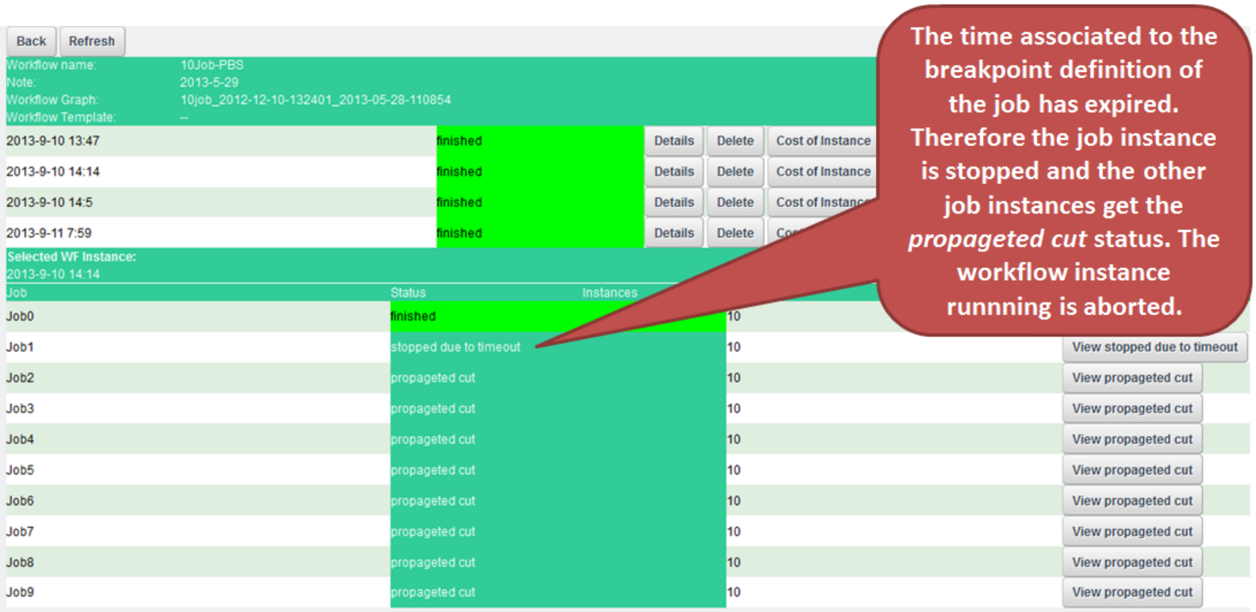
Workflow name: JavaTarball_64-EVAL_2013-06-24-072348_2013-07-09-093410
Note: 2012-2-1
Workflow Graph: javaAndTarball_2013-06-24-072348_2013-07-09-093410
Workflow Template: --

2013-9-5 12:6 finished

Selected WF Instance:
2013-9-5 12:6

Job	Status	Instances	[Actions]
Java	finished	1	View finished
FINAL-EVAL	finished	1	View finished
TarBallTest	finished	1	View finished

Figure 13.7 The effect of enabling run a job instance.


Back
Refresh
Details
Delete
Cost of Instance

Workflow name: 10Job-PBS
Note: 2013-5-29
Workflow Graph: 10job_2012-12-10-132401_2013-05-28-110854
Workflow Template: --

2013-9-10 13:47	finished	Details Delete Cost of Instance
2013-9-10 14:14	finished	Details Delete Cost of Instance
2013-9-10 14:5	finished	Details Delete Cost of Instanc
2013-9-11 7:59	finished	Details Delete Co

Selected WF Instance:
2013-9-10 14:14

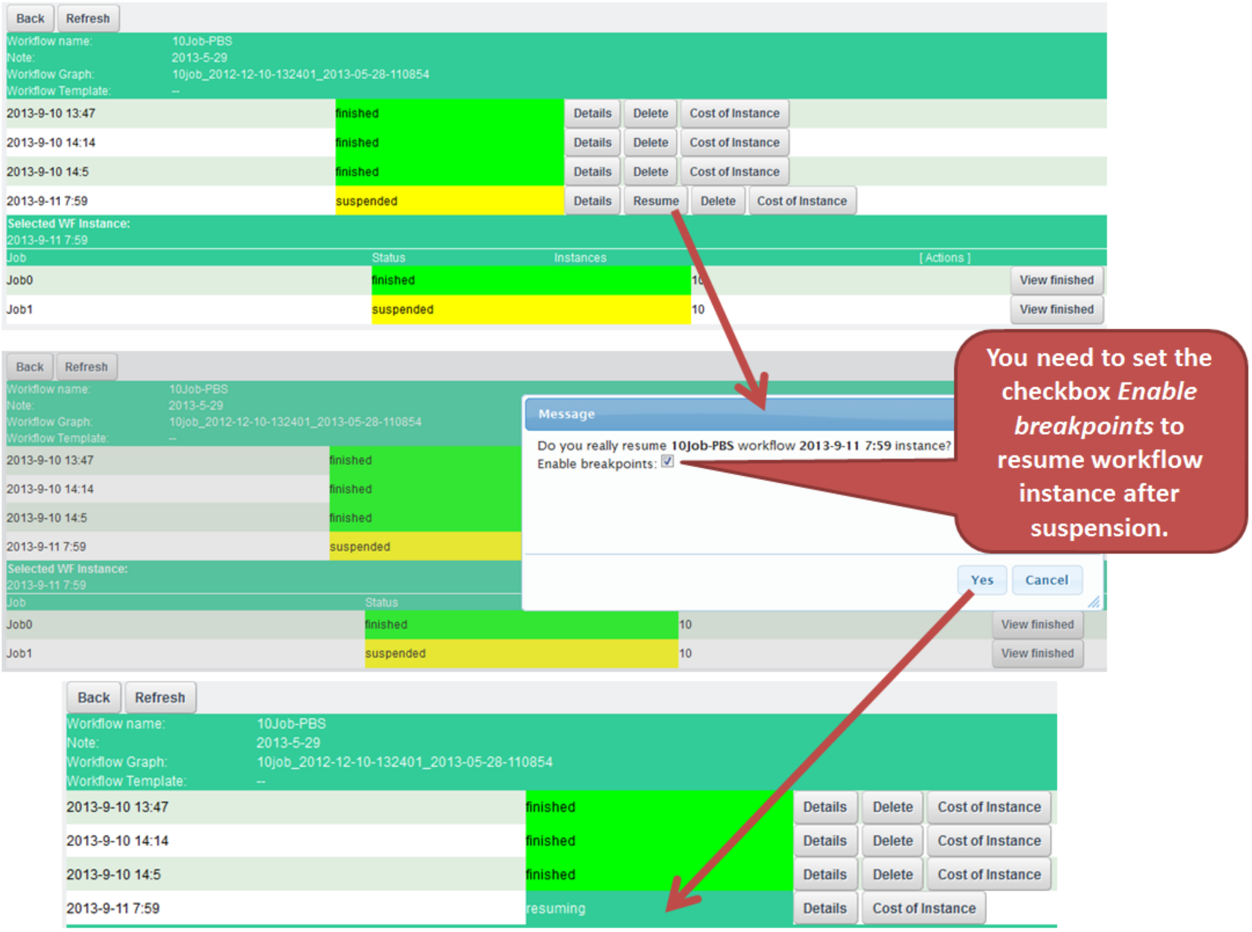
Job	Status	Instances	
Job0	finished	10	
Job1	stopped due to timeout	10	View stopped due to timeout
Job2	propageted cut	10	View propageted cut
Job3	propageted cut	10	View propageted cut
Job4	propageted cut	10	View propageted cut
Job5	propageted cut	10	View propageted cut
Job6	propageted cut	10	View propageted cut
Job7	propageted cut	10	View propageted cut
Job8	propageted cut	10	View propageted cut
Job9	propageted cut	10	View propageted cut

The time associated to the breakpoint definition of the job has expired. Therefore the job instance is stopped and the other job instances get the *propageted cut* status. The workflow instance runnning is aborted.

Figure 13.8 A workflow instance details in case of expired waiting time at a breakpoint

Advanced debugging facilities: suspension and subsequent resume operations issued on a running workflow instance modify the states all job instances which are in a transient or error state. Between “suspend” and “resume” the user may redefine the breakpoint configuration of the related workflow. The marking of the *Enable breakpoints* check box visible in popup menu for the confirmation of the issued “resume” operation activates debug regime (see Fig. 13.9).

Warning: When job instances of a workflow configured with “Before submission” option reach during workflow instance running the defined breakpoint, and when you changes at this point the configurations (e.g. command line arguments) of this breakpointed jobs, then the job instances resume running after breakpoint with the old configurations (the changes won’t be realized). To enforce indeed the changes, you must use *Suspend* function before configuration changes and then the *Resume* function for your workflow.



Workflow name: 10Job-PBS
Note: 2013-5-29
Workflow Graph: 10job_2012-12-10-132401_2013-05-28-110854
Workflow Template: --

2013-9-10 13:47	finished
2013-9-10 14:14	finished
2013-9-10 14:5	finished
2013-9-11 7:59	suspended

Selected WF Instance:
2013-9-11 7:59

Job	Status	Instances	[Actions]
Job0	finished	10	View finished
Job1	suspended	10	View finished

Message

Do you really resume **10Job-PBS** workflow **2013-9-11 7:59** instance?
Enable breakpoints: ☑

You need to set the checkbox *Enable breakpoints* to resume workflow instance after suspension.

Workflow name: 10Job-PBS
Note: 2013-5-29
Workflow Graph: 10job_2012-12-10-132401_2013-05-28-110854
Workflow Template: --

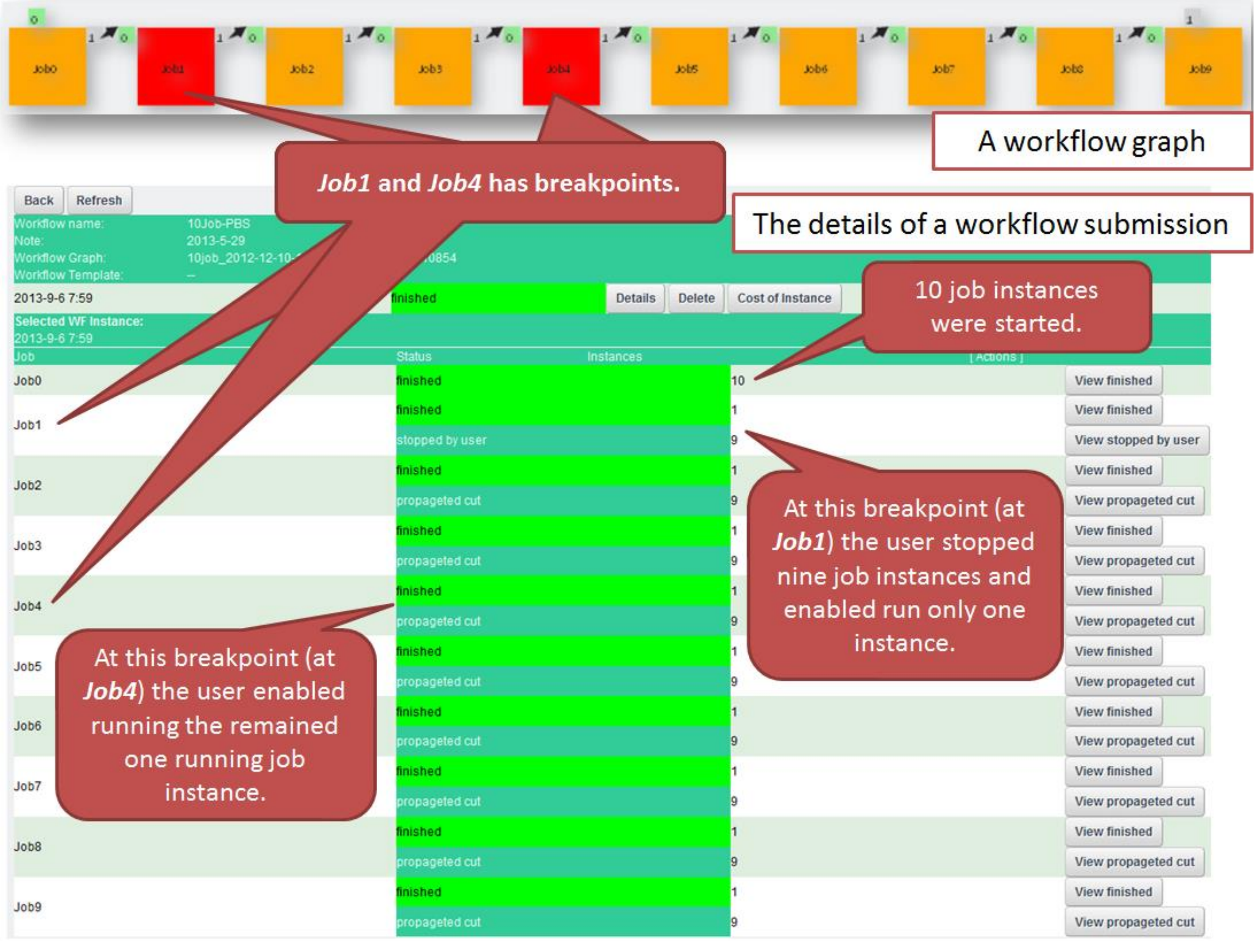
2013-9-10 13:47	finished
2013-9-10 14:14	finished
2013-9-10 14:5	finished
2013-9-11 7:59	resuming

Figure 13.9 Enabling breakpoints to resume workflow instance running after suspension

The next example demonstrates the effect of the debugging related new job states on the overall progress of workflow interpretation: (see Fig. 13.10). Two jobs are associated with breakpoints during workflow configuration, and the workflow is feed by a PS set of 10 members. (See the upper part of the figure.)

The lower part of the figure ("Details" view of the workflow submission) reveals that the user has enabled the progress of just 1 instance of the set has been stopped by the breakpoint at "Job1" and has enabled later the progress of the single job instance, which has been stopped by the breakpoint at "Job4".

Warning: breakpoint configuration and the workflow submission in debugging regime are not available in **end-user mode**.



Job1 **and** ***Job4*** **has breakpoints.**

Workflow name: 10Job-PBS
Note: 2013-5-29
Workflow Graph: 10job_2012-12-10-
Workflow Template: –

2013-9-6 7:59 finished

Selected WF Instance:
2013-9-6 7:59

Job	Status	Instances	[Actions]
Job0	finished	10	View finished
Job1	finished	1	View finished
	stopped by user	9	View stopped by user
Job2	finished	1	View finished
	propageted cut	9	View propagated cut
Job3	finished	1	View finished
	propageted cut	9	View propagated cut
Job4	finished	1	View finished
	propageted cut	9	View propagated cut
Job5	finished	1	View finished
	propageted cut	9	View propagated cut
Job6	finished	1	View finished
	propageted cut	9	View propagated cut
Job7	finished	1	View finished
	propageted cut	9	View propagated cut
Job8	finished	1	View finished
	propageted cut	9	View propagated cut
Job9	finished	1	View finished
	propageted cut	9	View propagated cut

10 job instances were started.

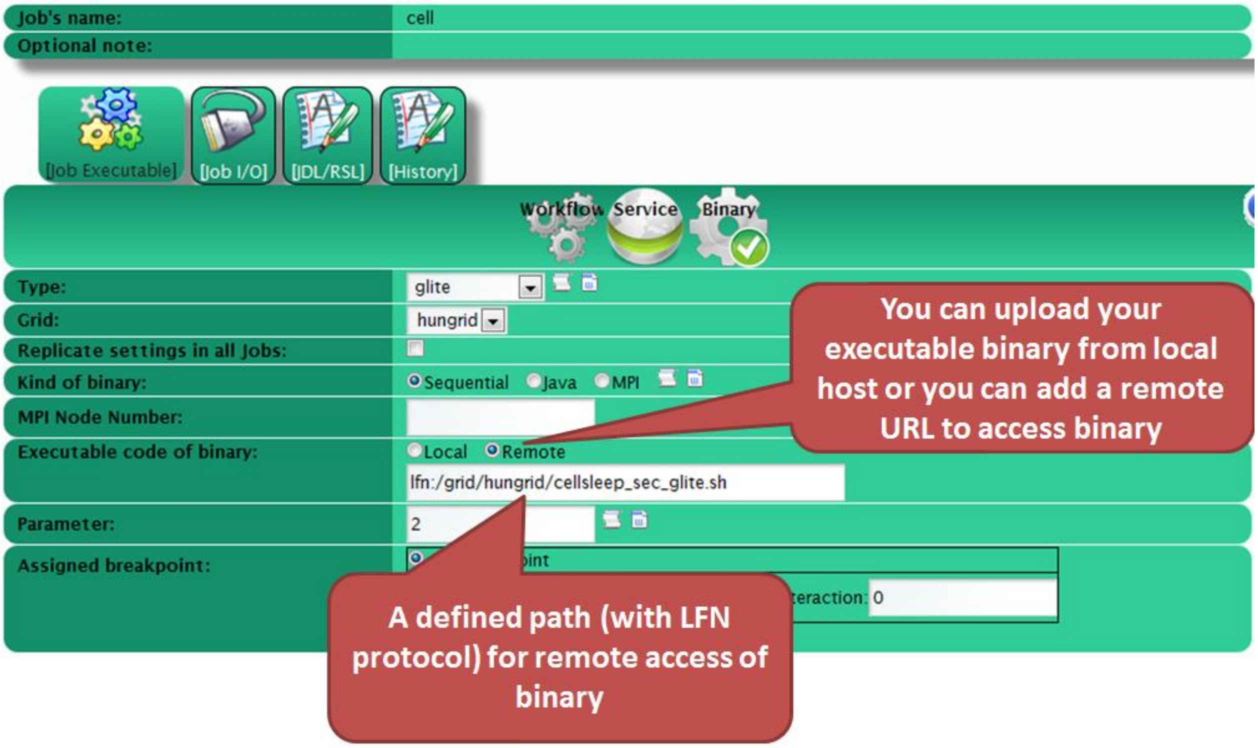
At this breakpoint (at ***Job1***) the user stopped nine job instances and enabled run only one instance.

At this breakpoint (at ***Job4***) the user enabled running the remained one running job instance.

Figure 13.10 A details view of a ten-job workflow instance submission

14. Defining Remote Executable and Input

During the job configuration process you need to define your executable code of binary within the *Concrete/Job Executable* tab (Figure 14.1). You can do it not only by uploading binary from your local machine (*Local* option) but by adding the corresponding remote path of the executable (*Remote* option).



Job's name: cell

Optional note:

Type: glite

Grid: hungrid

Replicate settings in all Jobs: ☐

Kind of binary: ● Sequential ○ Java ○ MPI

MPI Node Number:

Executable code of binary: ○ Local ● Remote

lfn:/grid/hungrid/cellsleep_sec_glite.sh

Parameter: 2

Assigned breakpoint:

You can upload your executable binary from local host or you can add a remote URL to access binary

A defined path (with LFN protocol) for remote access of binary

Figure 14.1 Remote option in the Executable code of binary setting within the Job Executable tab

You can use the *Remote* option to the following Grid *Types* together with the next protocols for the *Executable code of binary* definition:

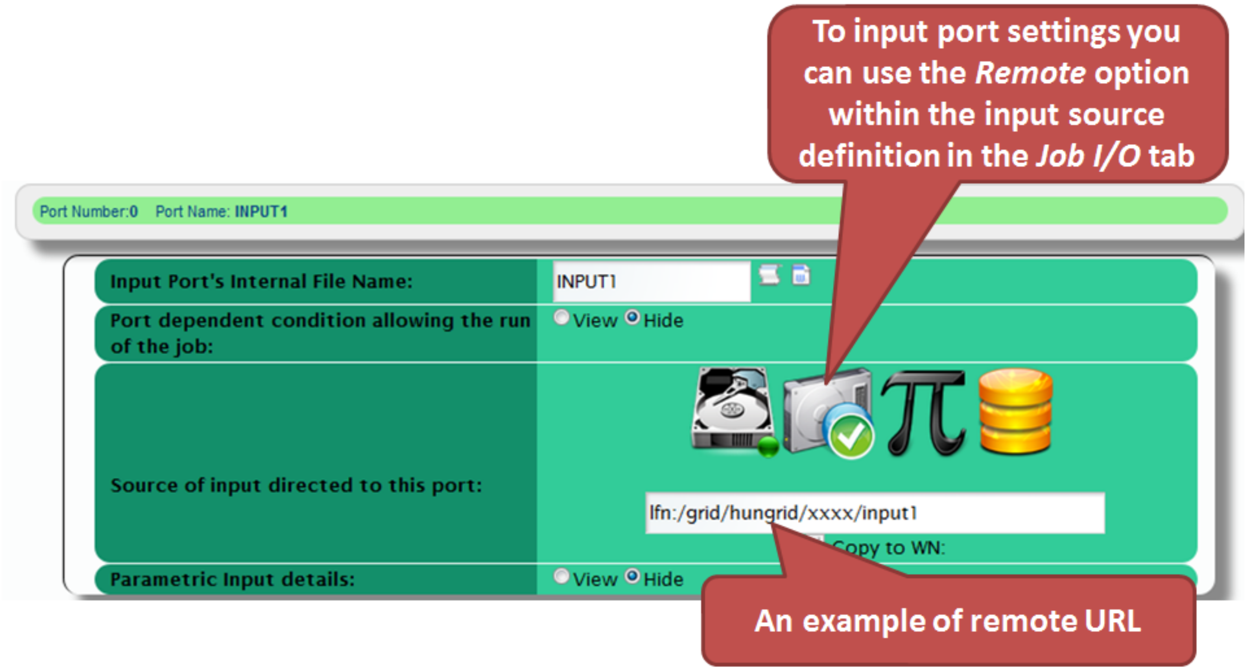
Grid Type	Supported Protocols
gLite	file, http, lfn
GT2	file, http, gsiftp
GT4	file, http, gsiftp
GT5	file, http, gsiftp
UNICORE	http, idbtool
ARC	http

LSF	http
PBS, SGE	file, http
Local	file, http

Warning: You can't add **robot permission association** in case of applying remote executable. (For more details about robot permission, see chapter 20 within Menu-Oriented Online-Help.)

You can also use the *Remote* option (by selecting the "*Remote*" icon) to input port definition within the *Concrete/Job I/O* tab (Figure 14.2). In this case you can use the following Grid Types and protocols:

Grid Type	Supported Protocols
gLite	http, lfn
GT2	http, gsiftp
GT4	http, gsiftp
GT5	http, gsiftp
UNICORE	http, xtreemfs
ARC	http
LSF	http
PBS	http
Local	http


Port Number:0 Port Name: INPUT1

Input Port's Internal File Name: INPUT1

Port dependent condition allowing the run of the job: ○ View ● Hide

Source of input directed to this port: lfn:/grid/hungrid/xxxx/input1

Copy to WN:

Parametric Input details: ○ View ● Hide

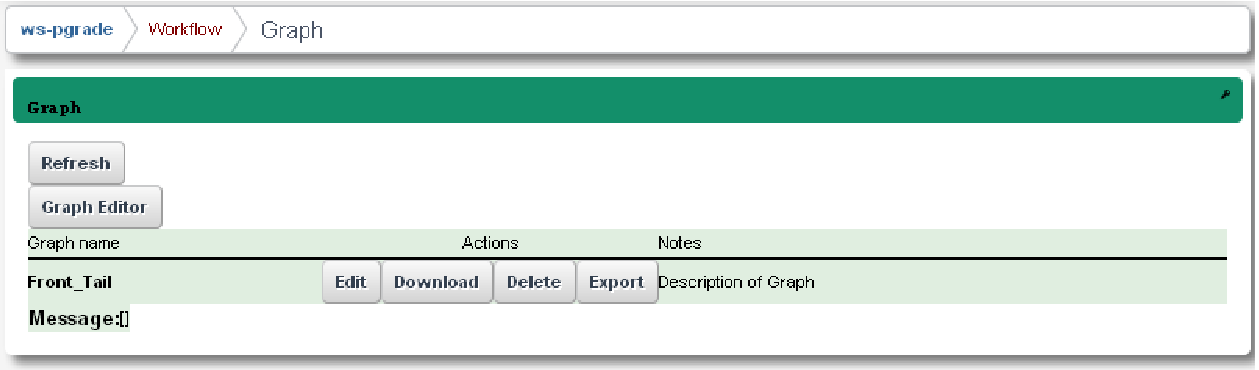
To input port settings you can use the *Remote* option within the input source definition in the *Job I/O* tab

An example of remote URL

Figure 14.2 Remote source setting to input port within the Job I/O tab

Menu-Oriented Online Help (Appendix I)

1. The Graph Menu



Front_Tail — Description of Graph

Message:[]

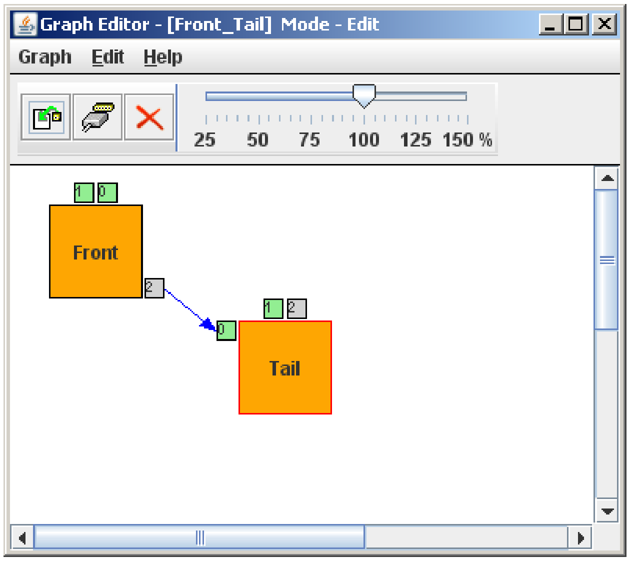
Appendix Figure 1 Graph menu

This tab serves the management of workflow Graphs. Graphs are created and modified by the Graph Editor.

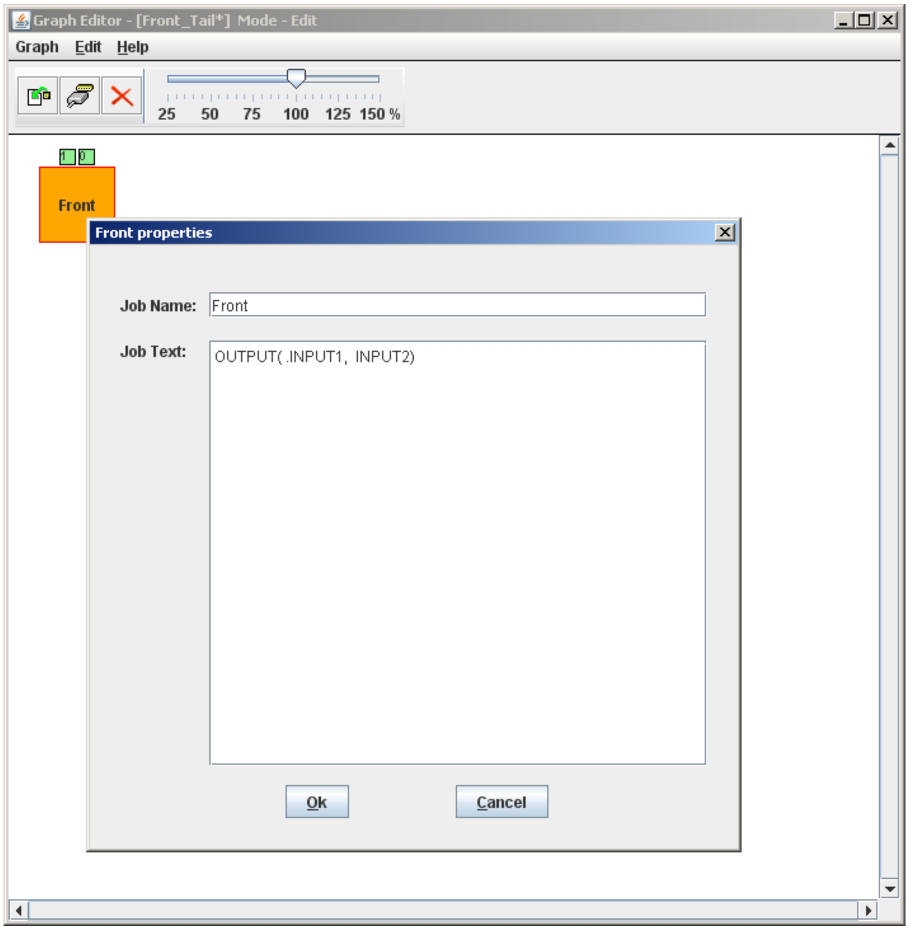
The *Graph Editor* (see Appendix Figure 2) runs on the user's desktop in a separate window dedicated to the given Graph object. The *Graph Editor* can be called

- either by clicking on the Graph Editor button – for example to create a new Graph,
- or by clicking on the button Edit for example in the case when the user wants to modify, or copy an existing Graph.

An existing graph can be downloaded to the user's desktop machine by pressing the *Download* button. A subsequent upload can be done in the *Workflow/Upload* tab. The user can change the name of the graph which he/she wants to upload. The graph objects of the user have a common namespace (with the exception of embedded workflows graphs within projects and applications). The name collision is detected and prohibited. Clicking on the *Delete* button the user deletes the graph object from the graph list. Clicking on the *Export* button the user uploads the graph object in a repository, common among all Users. A subsequent reload from the repository can be done on the tab *Workflow/Import*. The *Refresh* button serves the synchronization: All existing graph objects (their list is extended by the saved products of the *Graph Editors*, running parallel on the user's desktop machine) are listed.


Graph Editor - [Front_Tail] Mode - Edit
Graph
Edit
Help
25
50
75
100
125
150 %
1
0
Front
2
1
2
0
Tail

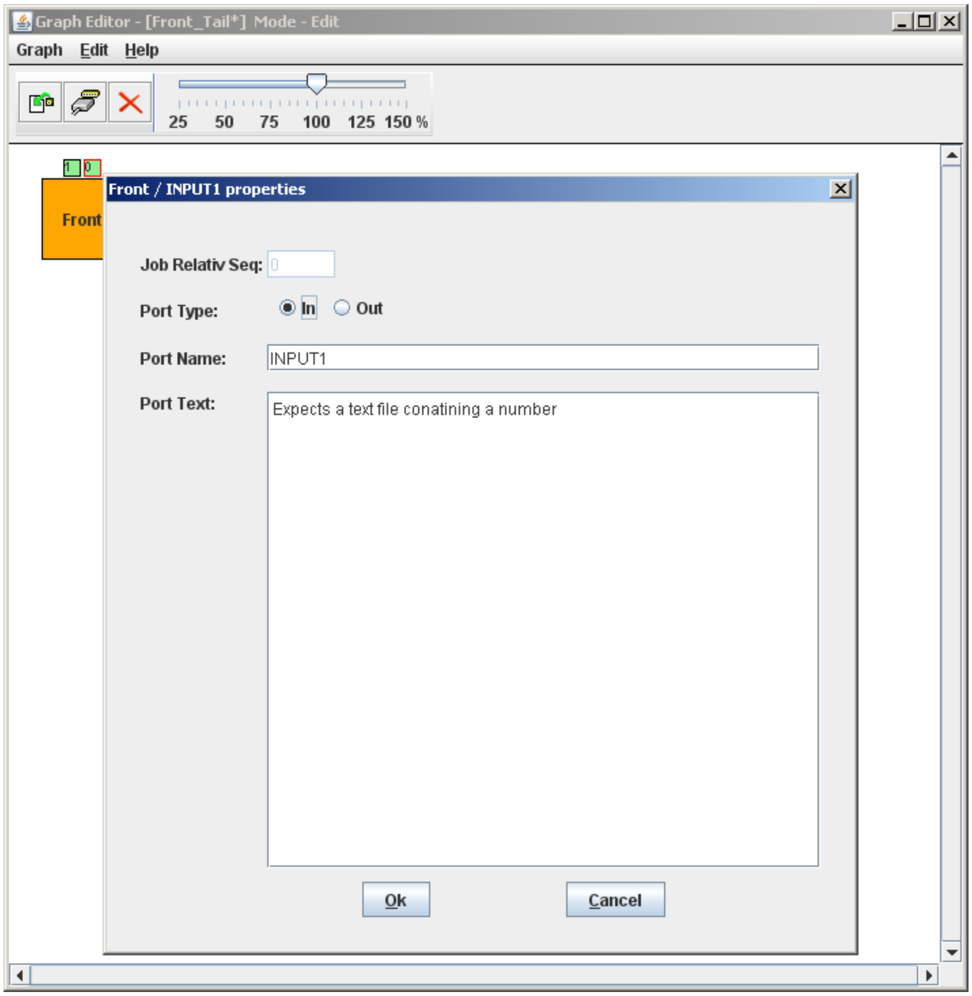
Appendix Figure 2 Graph Editor main view


Graph Editor - [Front_Tail*] Mode - Edit
Graph
Edit
Help
25
50
75
100
125
150 %
1
0
Front
Front properties
Ok
Cancel

Job Name: Front

Job Text: OUTPUT(.INPUT1, INPUT2)

Appendix Figure 3 Graph Editor Job properties


Graph Editor - [Front_Tail*] Mode - Edit
Graph
Edit
Help
25
50
75
100
125
150 %
Front
Front / INPUT1 properties
Ok
Cancel

Job Relativ Seq: 0

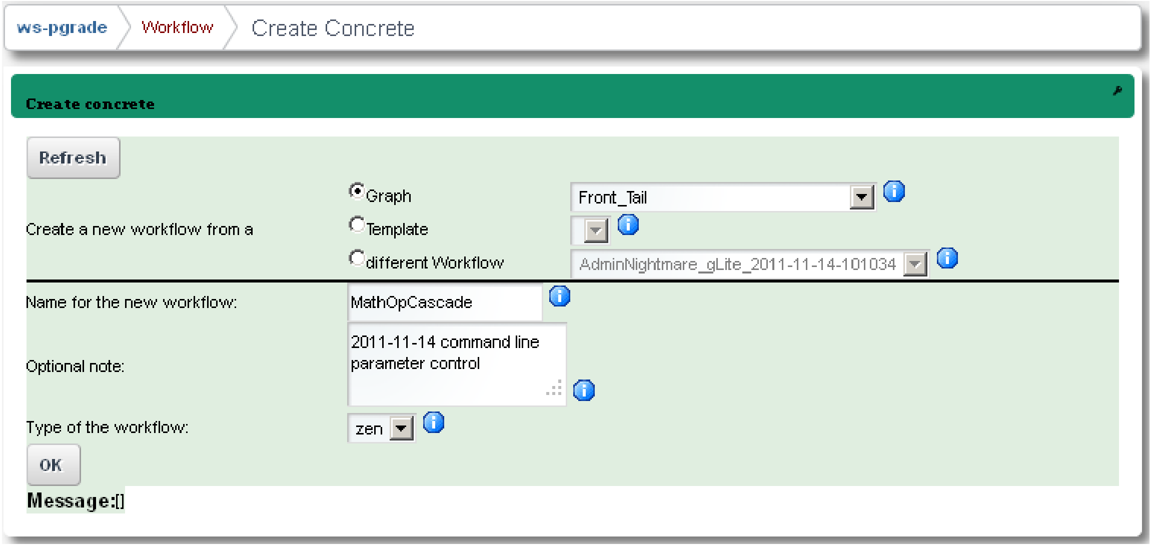
Port Type: ● In ○ Out

Port Name: INPUT1

Port Text: Expects a text file conatining a number

Appendix Figure 4 Graph Editor, Port properties

2. The Create Concrete Menu



Create a new workflow from a ● Graph Front_Tail
○ Template
○ different Workflow AdminNightmare_gLite_2011-11-14-101034

Name for the new workflow: MathOpCascade

Optional note: 2011-11-14 command line parameter control

Type of the workflow: zen

Message:[]

Appendix Figure 5 Creation of a new workflow

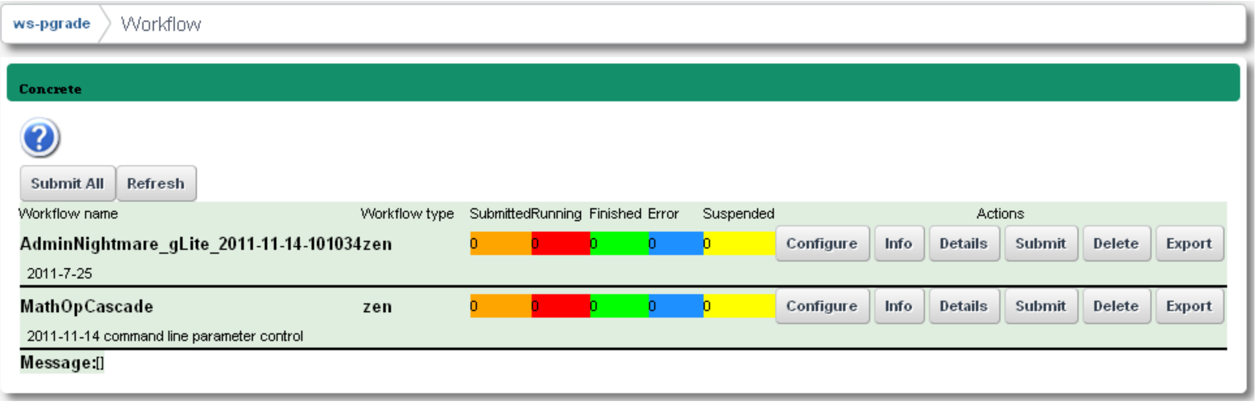
A new workflow can be defined on this tab. A workflow explicitly or implicitly must reference a graph. The user selects the root of the workflow generation by the radio button Create a new workflow from a.

Depending on the choice an existing graph, an existing template (referencing already a graph) or an existing different workflow (also referencing a graph) can be used to create a new Workflow with a user defined name and with a user defined *Optional note*.

The configuration of the created workflow can be performed in the *Workflow/Concrete* tab by clicking the *Configure* button in the line belonging to the created Workflow. By giving the Name for the new workflow please note that the workflows and templates have a common namespace and all entries must be called differently. *OK* button closes and confirms the creation.

The *Refresh* button serves the synchronization: All existing graph objects (whose list will be extended by the saved products of the *Graph Editor* running parallel on the user's desktop machine) will be listed in the checklist belonging to the graph selector. The *Type of the workflow* list box is reserved for later use in order to select a workflow enactor. The default enactor is the "*zen*".

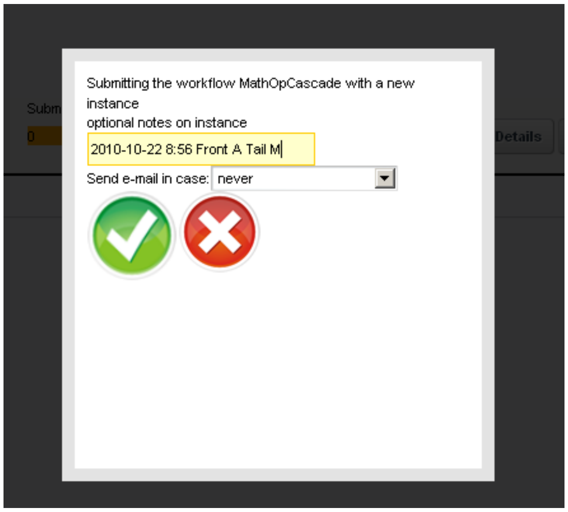
3. The Concrete Menu



Workflow name	Workflow type	Submitted	Running	Finished	Error	Suspended	Actions
AdminNightmare_gLite_2011-11-14-101034 2011-7-25	zen	0	0	0	0	0	Configure Info Details Submit Delete Export
MathOpCascade 2011-11-14 command line parameter control	zen	0	0	0	0	0	Configure Info Details Submit Delete Export

Message:[]

Appendix Figure 6 Main view of the Concrete menu



Submitting the workflow MathOpCascade with a new instance

optional notes on instance

2010-10-22 8:56 Front A Tail M

Send e-mail in case: never

Appendix Figure 7 Workflow submit

This tab lists the configurable and ready to submit workflows owned by the given user. Workflows listed here are either have been created in the *Workflow/Create* tab or have been uploaded from the user's desktop machine using tab Workflow/Upload or have been imported from the central Repository using the *Workflow/Import* tab. These workflows are either fully configured according to the will of the user or their semantics must be defined or altered. (I.)

In case of fully configured workflows the user can submit them if there is a proper proxy certificate (obtainable in the tab *Certificates/Download*) to all requested Grid resources requested by the workflow. The user can control the fully qualified and ready to submit state of the workflow by the button Info listing the eventual undefined features/settings of the given workflow. For the time being this test does not includes the eventual problems of the embedded workflows as these objects will be activated run time. A correct workflow can be submitted by using the button Submit. Upon submission a new object, the Workflow Instance will be created.

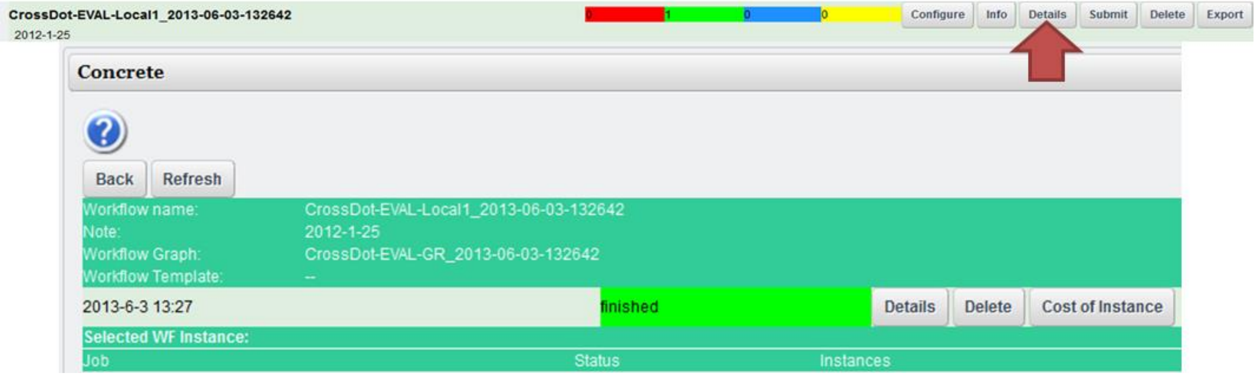
The workflow instance contains additional information (state of the workflow Instance, among others the created log and output files). During the obligatory submission conforming process the user may add a comment in order to distinguish the different workflow instances having been created manually. This called direct submission. Indirect submission occurs if a given workflow has been mentioned in a job configuration to interpret the semantics of that job (embedded workflow). During the execution of the workflow containing the mentioned job, upon elaborating that job the workflow interpreter executes this "call" as a new workflow submission with the consequence that a new Workflow Instance will be created from the embedded workflow. However, in this case an automatically created unique label will distinguish this workflow instance from the others.

The instances of the embedded workflows can be reached as if they would be the instances of common workflows. It follows that the workflows used for embedding must be also defined (fully qualified) and present on this workflow list. The *Details* button opens a window where all existing Instances of the workflow are enumerated and ready for more detailed analysis and manipulations. On the associated state statistics table the total number of the instances of a given workflow is subdivided in four categories according their run time states: *Submitted, Running, Finished, Error*.

By the *Suspend* button all instances of a given workflow can be suspended. (Suspended workflow instances can be resumed individually applicable in a sub window which may be opened by the *Details* button.) A workflow can be deleted with all of its instances by using the *Delete* button. A workflow can be exported in the (among the users common) Repository by using the *Export* button.

The *Configure* button opens the root of the workflow configuration window, where the graph of the workflow appears, and clicking on a job or on a port icon belonging to a job the proper item can be defined/modified.

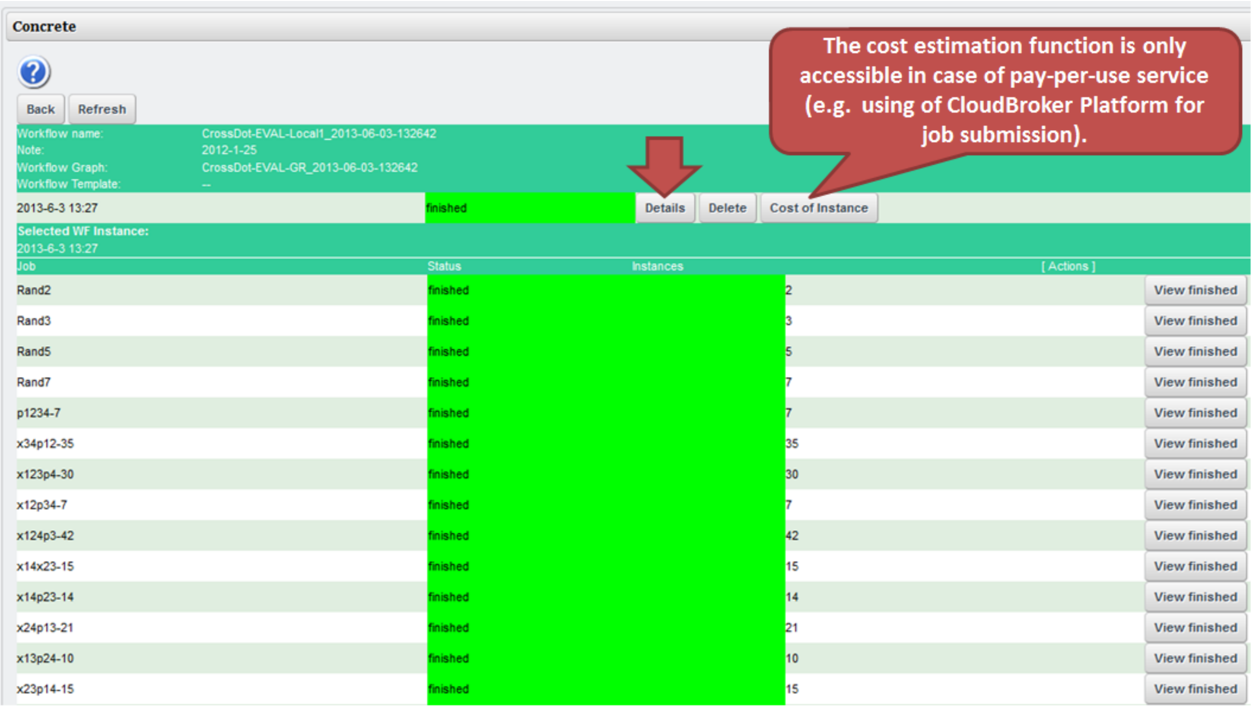
3.1 The Concrete/Details Function


CrossDot-EVAL-Local1_2013-06-03-132642
2012-1-25

Workflow name: CrossDot-EVAL-Local1_2013-06-03-132642
Note: 2012-1-25
Workflow Graph: CrossDot-EVAL-GR_2013-06-03-132642
Workflow Template: --

2013-6-3 13:27 finished

Appendix Figure 8 View of a workflow instance by the Concrete/Details function



The cost estimation function is only accessible in case of pay-per-use service (e.g. using of CloudBroker Platform for job submission).

Workflow name: CrossDot-EVAL-Local1_2013-06-03-132642
Note: 2012-1-25
Workflow Graph: CrossDot-EVAL-GR_2013-06-03-132642
Workflow Template: --

2013-6-3 13:27 finished

Selected WF Instance:
2013-6-3 13:27

Job	Status	Instances	[Actions]
Rand2	finished	2	View finished
Rand3	finished	3	View finished
Rand5	finished	5	View finished
Rand7	finished	7	View finished
p1234-7	finished	7	View finished
x34p12-35	finished	35	View finished
x123p4-30	finished	30	View finished
x12p34-7	finished	7	View finished
x124p3-42	finished	42	View finished
x14x23-15	finished	15	View finished
x14p23-14	finished	14	View finished
x24p13-21	finished	21	View finished
x13p24-10	finished	10	View finished
x23p14-15	finished	15	View finished

Appendix Figure 9 View of a job instance list with statuses by the Concrete/Details/Details function

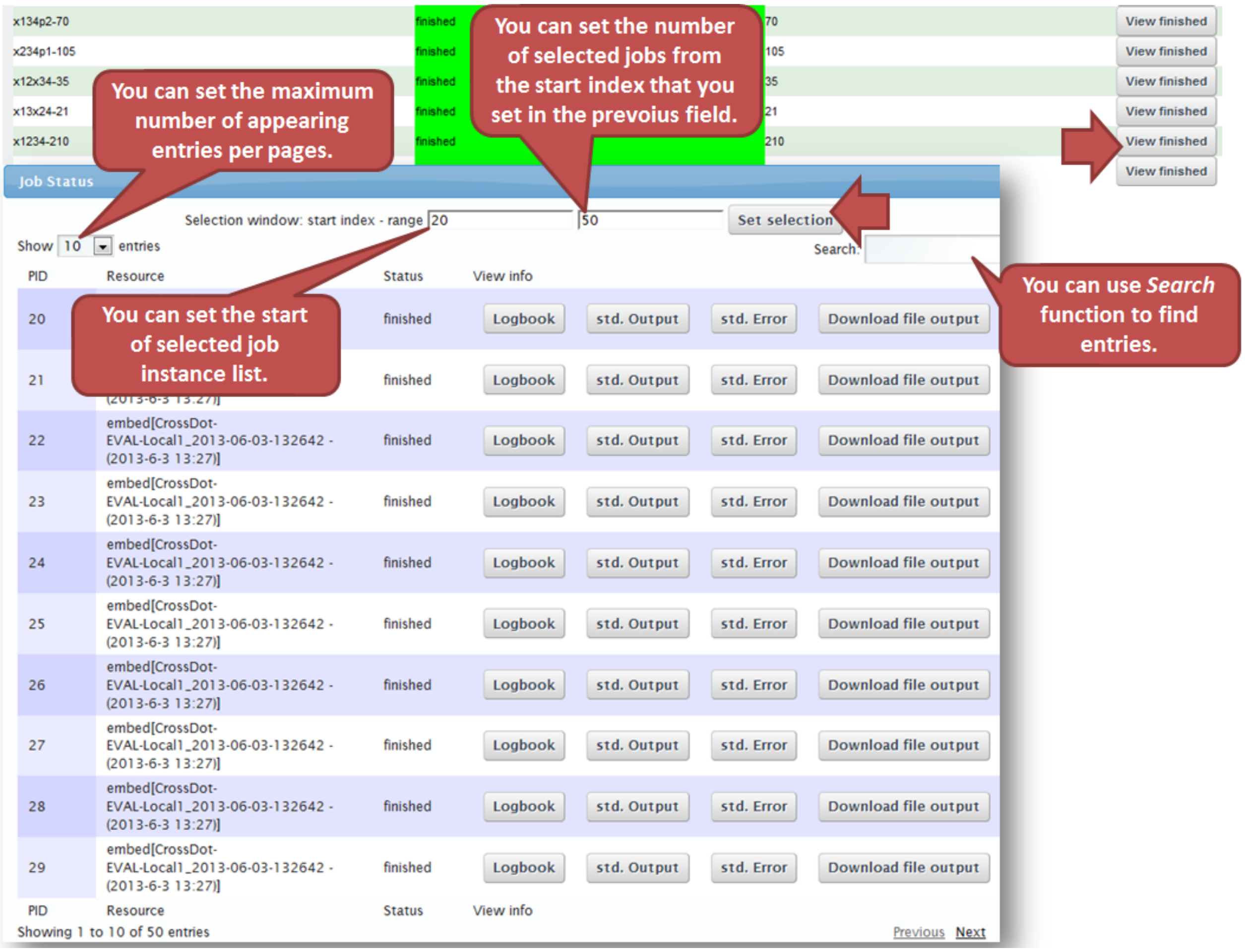
On this window the existing instances of the selected workflow are enumerated. They are ready for more detailed analysis and can be manipulated. The analysis can be done on a four level hierarchy where the encountering of the Instances is the root level. (Level 1)

From here the user can select to inspect the list of jobs belonging to the selected workflow instance (Level 2 reachable by button *Details*). There are two other buttons in this page: by *Delete* button you can delete the selected workflow instance view, and by *Cost of Instance* button you can access estimated cost information in case of pay-per-use workflow running service (currently, payment is necessary at CloudBroker-based job submission – see chapter 17 for details).

A single job may have several instances (and proper discriminating indices in their names) due to the fact, that the job may run several times within the control of a given workflow instance (if parameter sweep has been prescribed) creating a new job instance each time (Level 3. reachable by the button view *Content*(s)). Stepping even deeper in the hierarchy, the log and output files of a job instance can be reached (listed or downloaded) (Level 4, by the *Logbook, std. Output, std. Error, Download file output* buttons. On the workflow instance level (Level 1) the user can

- suspend/resume the Instance workflow by the toggle *Suspend/Resume* button,
- delete the workflow instance object by *Delete* button.

3.1.1 The Concrete/Details/Details/"View <Status>" Function



x134p2-70	finished	70	View finished
x234p1-105	finished	105	View finished
x12x34-35	finished	35	View finished
x13x24-21	finished	21	View finished
x1234-210	finished	210	View finished
			View finished

Job Status

Selection window: start index - range 20 50 Set selection

Show 10 entries

Search:

PID	Resource	Status	View info			
20		finished	Logbook	std. Output	std. Error	Download file output
21	(2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
22	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
23	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
24	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
25	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
26	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
27	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
28	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
29	embed[CrossDot-EVAL-Local1_2013-06-03-132642 - (2013-6-3 13:27)]	finished	Logbook	std. Output	std. Error	Download file output
PID	Resource	Status	View info			

Showing 1 to 10 of 50 entries

Previous Next

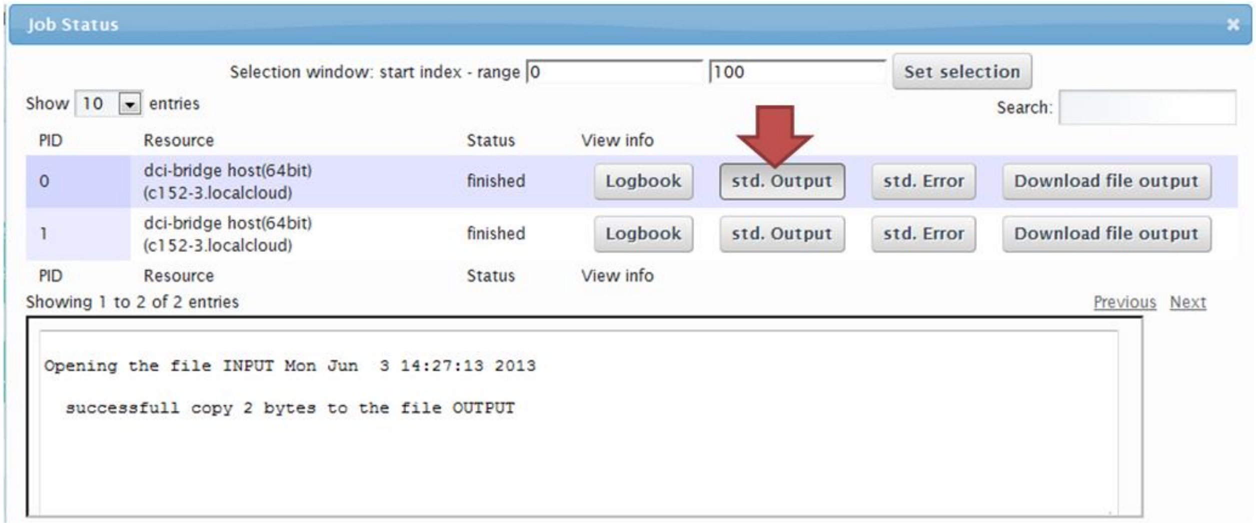
You can set the maximum number of appearing entries per pages.

You can set the number of selected jobs from the start index that you set in the prevoius field.

You can set the start of selected job instance list.

You can use *Search* function to find entries.

Appendix Figure 10 View job status details about instances of a “Finished” job submission



Job Status

Selection window: start index - range 0 100 Set selection

Show 10 entries

Search:

PID	Resource	Status	View info			
0	dci-bridge host(64bit) (c152-3.localcloud)	finished	Logbook	std. Output	std. Error	Download file output
1	dci-bridge host(64bit) (c152-3.localcloud)	finished	Logbook	std. Output	std. Error	Download file output
PID	Resource	Status	View info			

Showing 1 to 2 of 2 entries

Previous Next

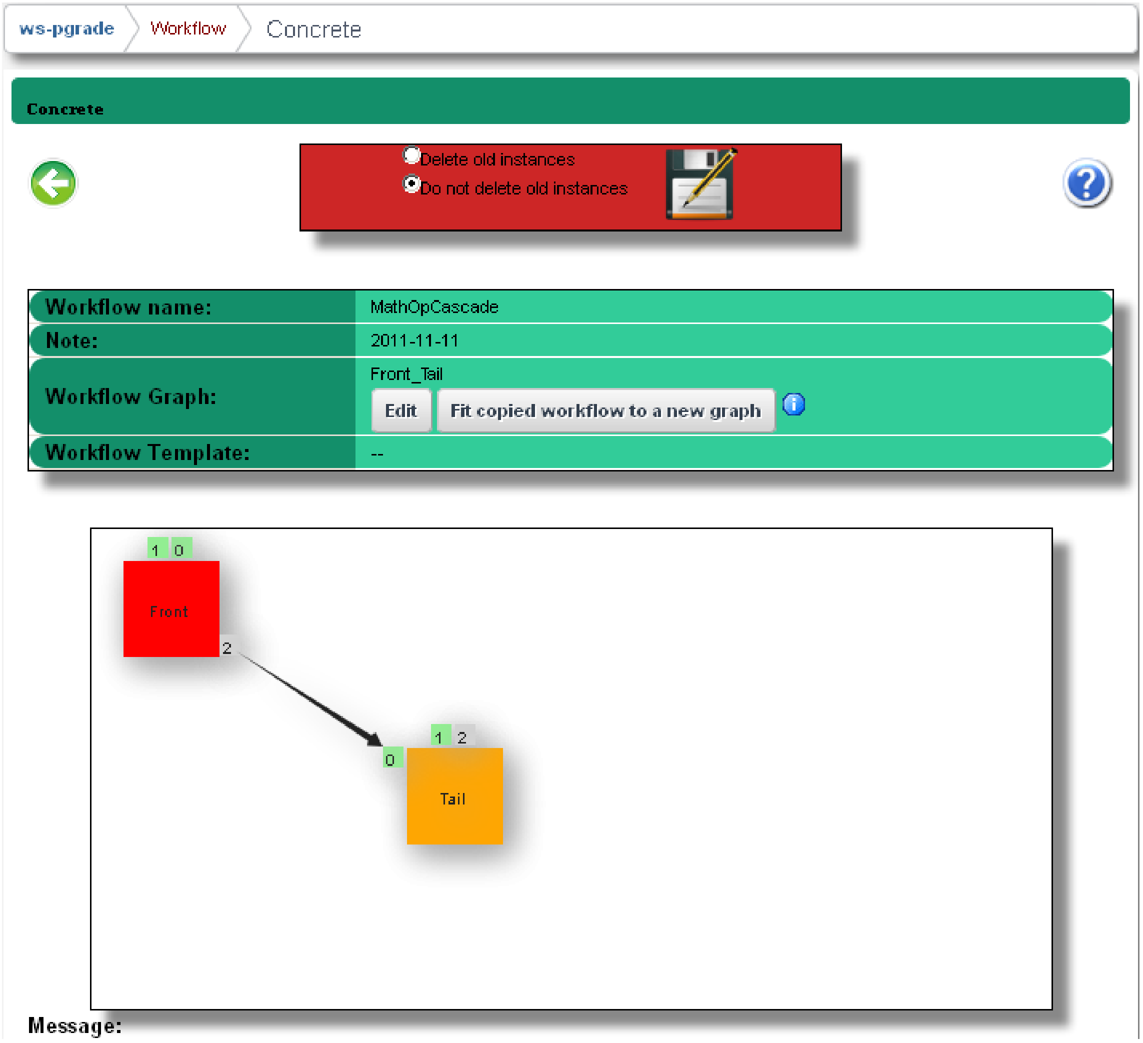
```
Opening the file INPUT Mon Jun  3 14:27:13 2013

  successfull copy 2 bytes to the file OUTPUT
```

Appendix Figure 11 View of the file "std. Output" of the selected job instance

On this level the log and output files of a job instance can be reached by *Logbook, std. Output, std. Error, Download file output* buttons, where the file output is a compressed file containing the local output files generated by the current run of the job.
The job instances are identified and listed with the following features:

- PID identifies the instance of the job which may be different from 0 in a Parameter Sweep running environment.
- Resource indicates the place where the job runs. Its content is submitter dependent and it may identify - for example - a Computing Element in case of job submissions of LCG2 or gLite type.
- Status informs about the current run time state of the job where the values of the state are submitter dependent but include the states init, submitted, finished, error.

3.2 The Concrete/Configure Menu



○ Delete old instances
● Do not delete old instances

Workflow name:	MathOpCascade
Note:	2011-11-11
Workflow Graph:	Front_Tail
Workflow Template:	--

Message:

Appendix Figure 12 Workflow configuration

This is the main window of the workflow configuration. The goal is to define - in a single or in several sessions – all the needed attributes which should be associated to the (in the beginning empty) jobs defined by the workflow graph in order to create a full defined, executable Workflow with a given semantics.

The workflow graph has been assigned to the workflow in the *Workflow/Create Concrete* tab. However, it is possible in the current menu to substitute the original graph with a new one. The reason behind this option is the possibility of the situation when the user wants modify the graph of the tested configured workflow and does not want to repeat the whole - sometimes tedious and error prone - configuration process. See details in Chapter 3.1.2.1.1.1.

The actual configuration can/must be done individually for each job. Either a job or a port belonging to a Job can be selected by clicking on its icon: A proper form will be opened, which must be filled and closed.

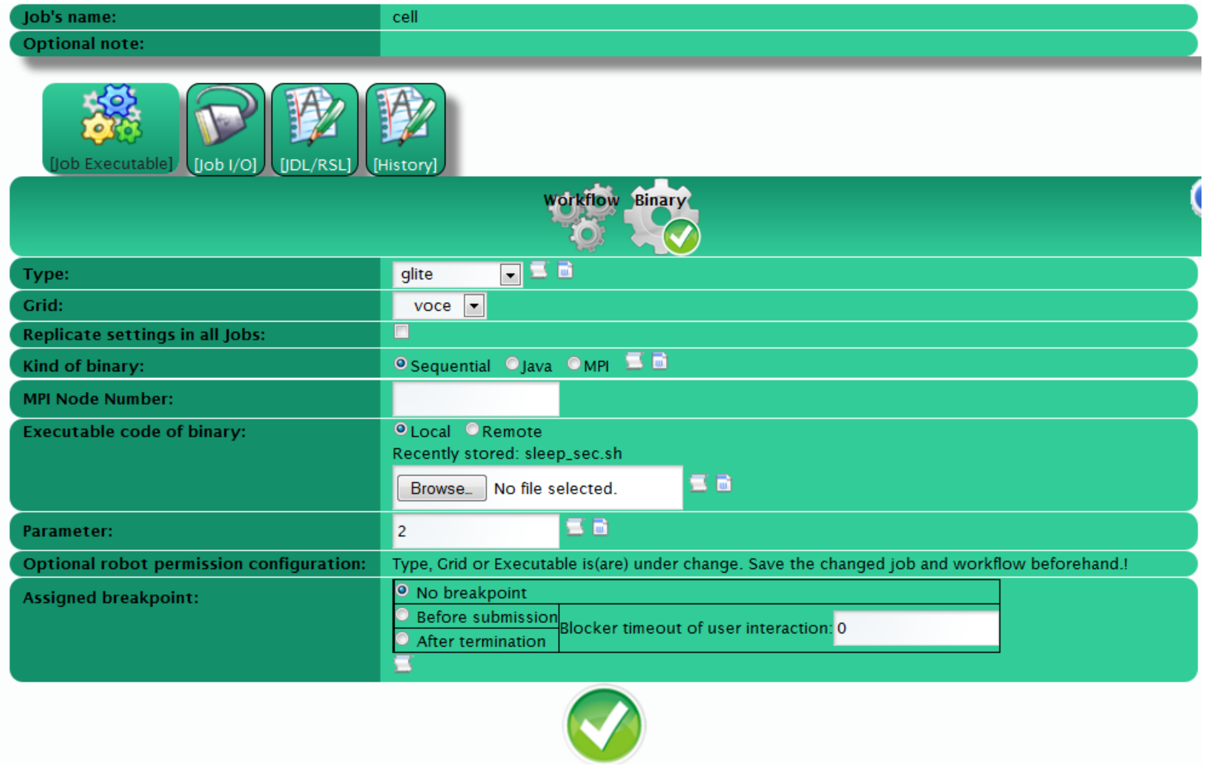
Note, that the configuration happens within the browser and the modifications will not be saved on the server until you close it by clicking on the *Save on Server* button.

Before doing that the user may decide by selecting the *Delete* radio button old instances to erase all eventual existing workflow instances belonging to the given workflow.

3.2.1 The Concrete/Configure/Job Executable Tab

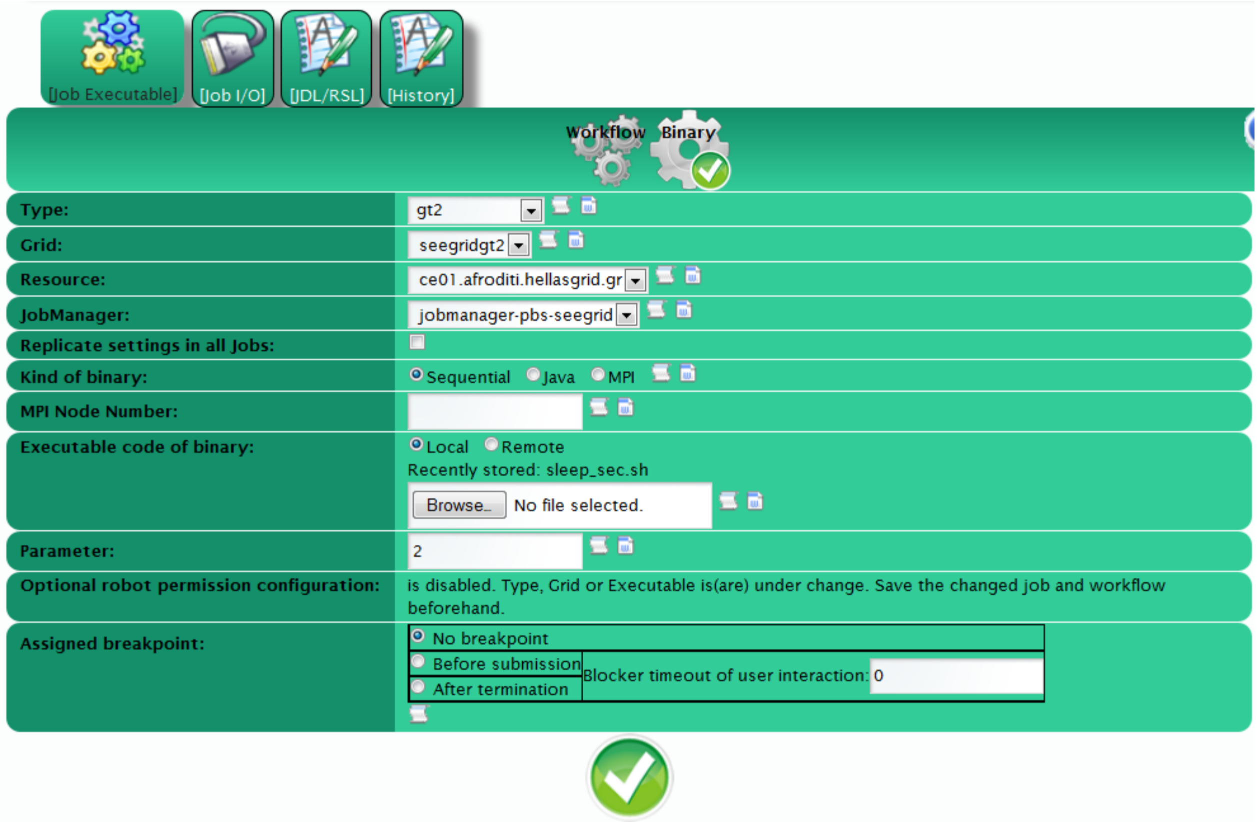
The *Job Executable* menu may appear in a different form depending on the selected regime which may be *Workflow, Service*, and *Binary*. The default regime is *Binary*. See Algorithm 2.1.

Within the *Binary* regime the *Type* determines the selected kind of middleware technology enumerated in the *Informations/Resources* menu.



Job's name:	cell
Optional note:	
Type:	glite
Grid:	voce
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	● Local ○ Remote Recently stored: sleep_sec.sh Browse... No file selected.
Parameter:	2
Optional robot permission configuration:	Type, Grid or Executable is(are) under change. Save the changed job and workflow beforehand.!
Assigned breakpoint:	● No breakpoint ○ Before submission ○ After termination Blocker timeout of user interaction: 0

Appendix Figure 13, Part A - gLite submitter


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Binary

Type: gt2

Grid: seegridgt2

Resource: ce01.afroditi.hellasgrid.gr

JobManager: jobmanager-pbs-seegrid

Replicate settings in all Jobs: ☐

Kind of binary: ● Sequential ○ Java ○ MPI

MPI Node Number:

Executable code of binary: ● Local ○ Remote

Recently stored: sleep_sec.sh

Browse... No file selected.

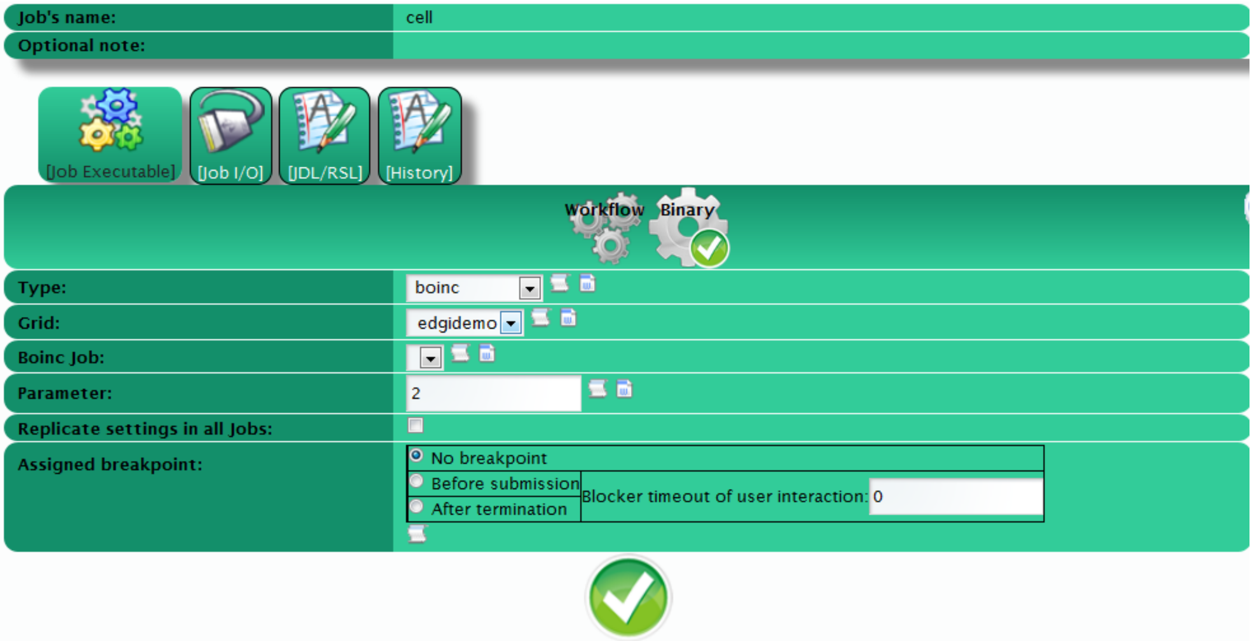
Parameter: 2

Optional robot permission configuration: is disabled. Type, Grid or Executable is(are) under change. Save the changed job and workflow beforehand.

Assigned breakpoint: ● No breakpoint ○ Before submission ○ After termination

Blocker timeout of user interaction: 0

Part B - gt2-gt4-gt5 submitter


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Binary

Job's name: cell

Optional note:

Type: boinc

Grid: edgidemo

Boinc Job:

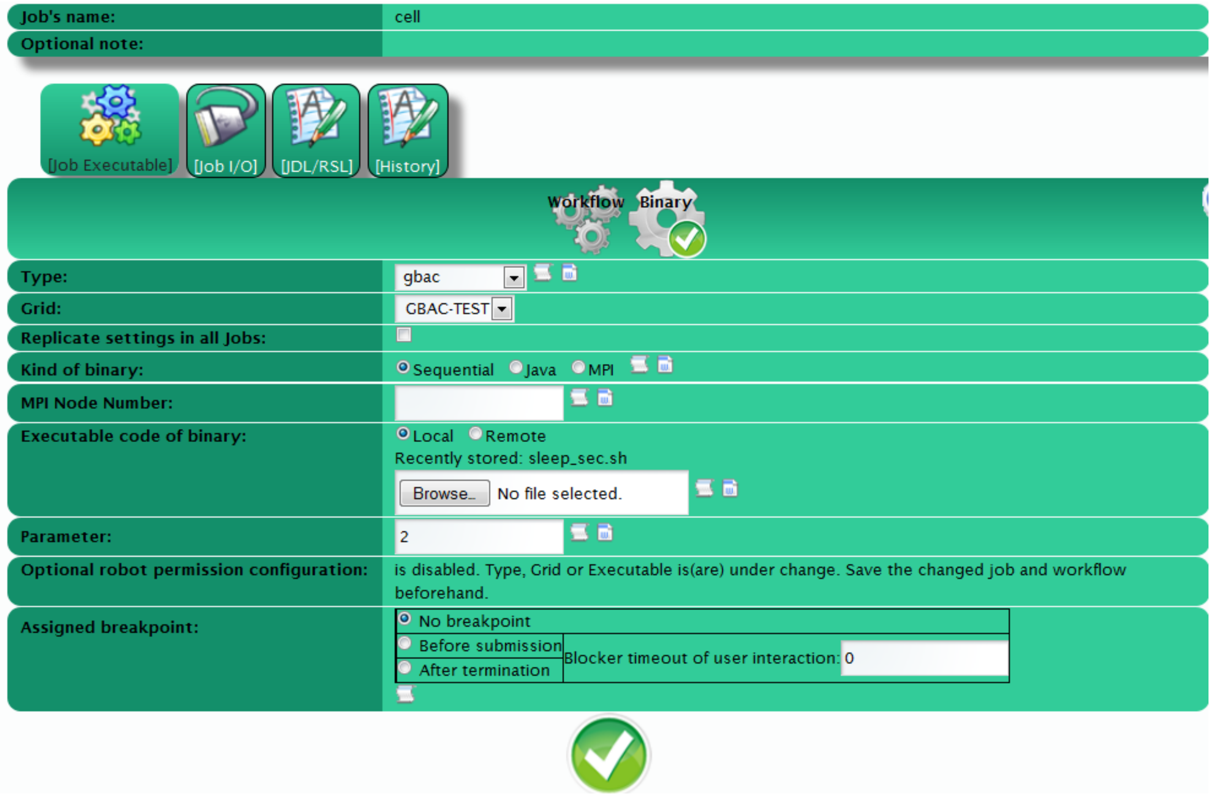
Parameter: 2

Replicate settings in all Jobs: ☐

Assigned breakpoint: ● No breakpoint ○ Before submission ○ After termination

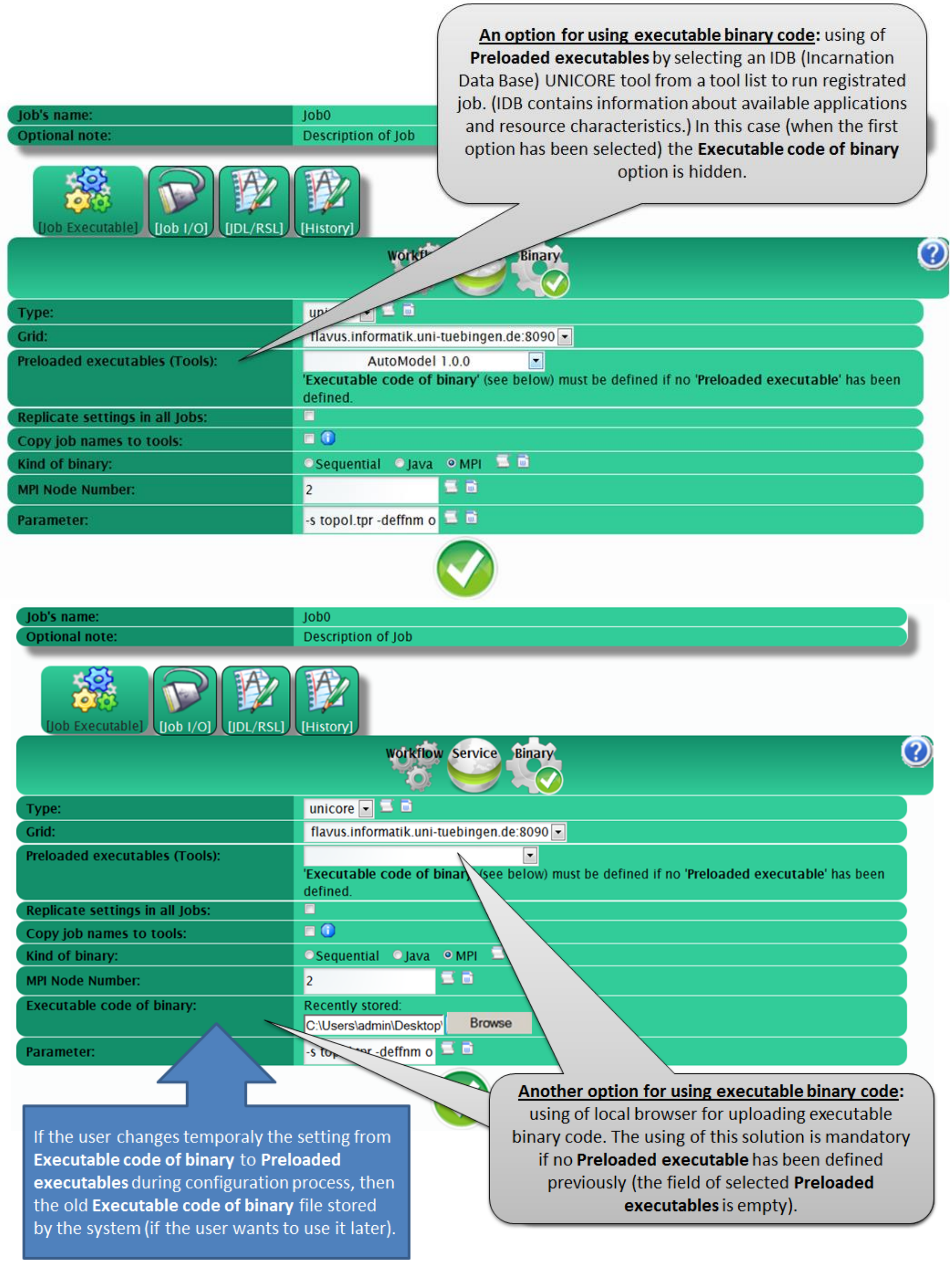
Blocker timeout of user interaction: 0

Part C BOINC configuration



Job's name:	cell
Optional note:	
Type:	gbac
Grid:	GBAC-TEST
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	● Local ○ Remote Recently stored: sleep_sec.sh Browse... No file selected.
Parameter:	2
Optional robot permission configuration:	is disabled. Type, Grid or Executable is(are) under change. Save the changed job and workflow beforehand.
Assigned breakpoint:	● No breakpoint ○ Before submission ○ After termination Blocker timeout of user interaction: 0

Part D GBAC configuration



An option for using executable binary code: using of **Preloaded executables** by selecting an IDB (Incarnation Data Base) UNICORE tool from a tool list to run registrated job. (IDB contains information about available applications and resource characteristics.) In this case (when the first option has been selected) the **Executable code of binary** option is hidden.

Job's name:	Job0
Optional note:	Description of Job

Type:	un
Grid:	flavus.informatik.uni-tuebingen.de:8090
Preloaded executables (Tools):	AutoModel 1.0.0 '**Executable code of binary**' (see below) must be defined if no '**Preloaded executable**' has been defined.
Replicate settings in all Jobs:	☐
Copy job names to tools:	☐
Kind of binary:	○ Sequential ○ Java ● MPI
MPI Node Number:	2
Parameter:	-s topol.tpr -deffnm o

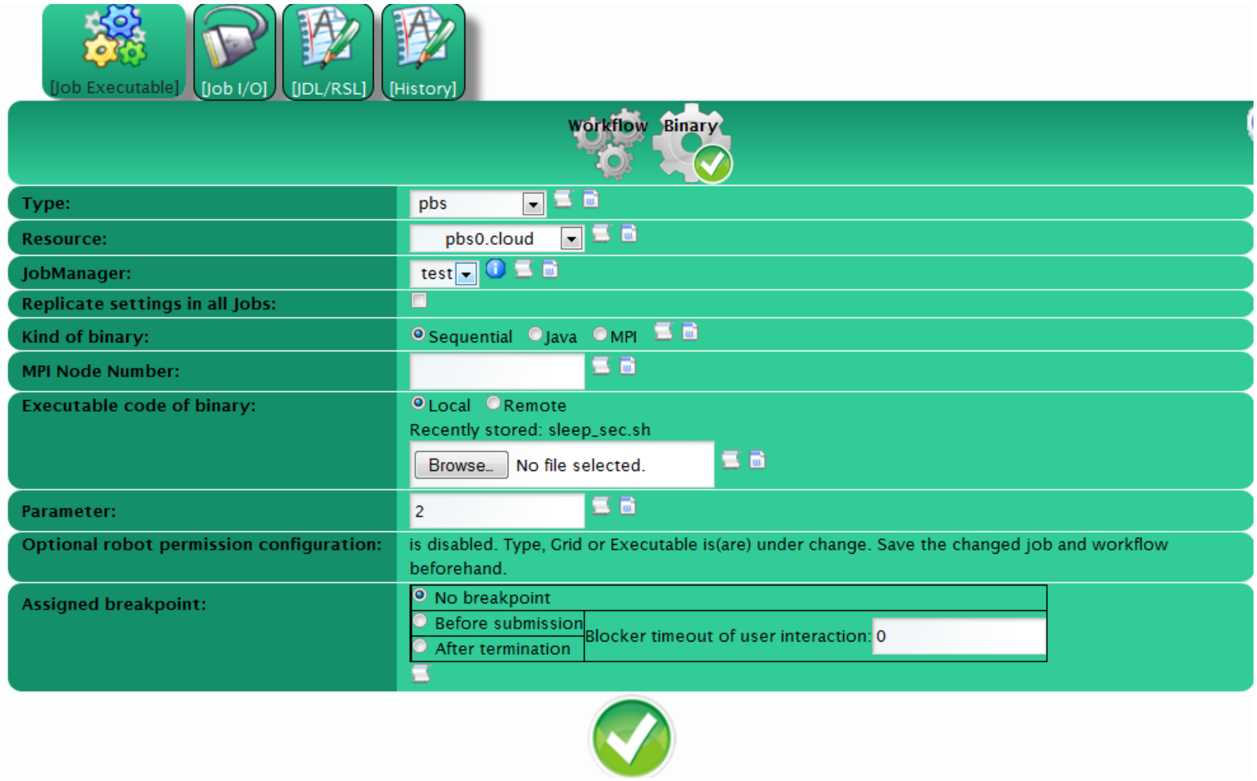
Job's name:	Job0
Optional note:	Description of Job

Type:	unicore
Grid:	flavus.informatik.uni-tuebingen.de:8090
Preloaded executables (Tools):	'**Executable code of binar** (see below) must be defined if no '**Preloaded executable**' has been defined.
Replicate settings in all Jobs:	☐
Copy job names to tools:	☐
Kind of binary:	○ Sequential ○ Java ● MPI
MPI Node Number:	2
Executable code of binary:	Recently stored: C:\Users\admin\Desktop\ Browse
Parameter:	-s to -deffnm o

If the user changes temporaly the setting from **Executable code of binary** to **Preloaded executables** during configuration process, then the old **Executable code of binary** file stored by the system (if the user wants to use it later).

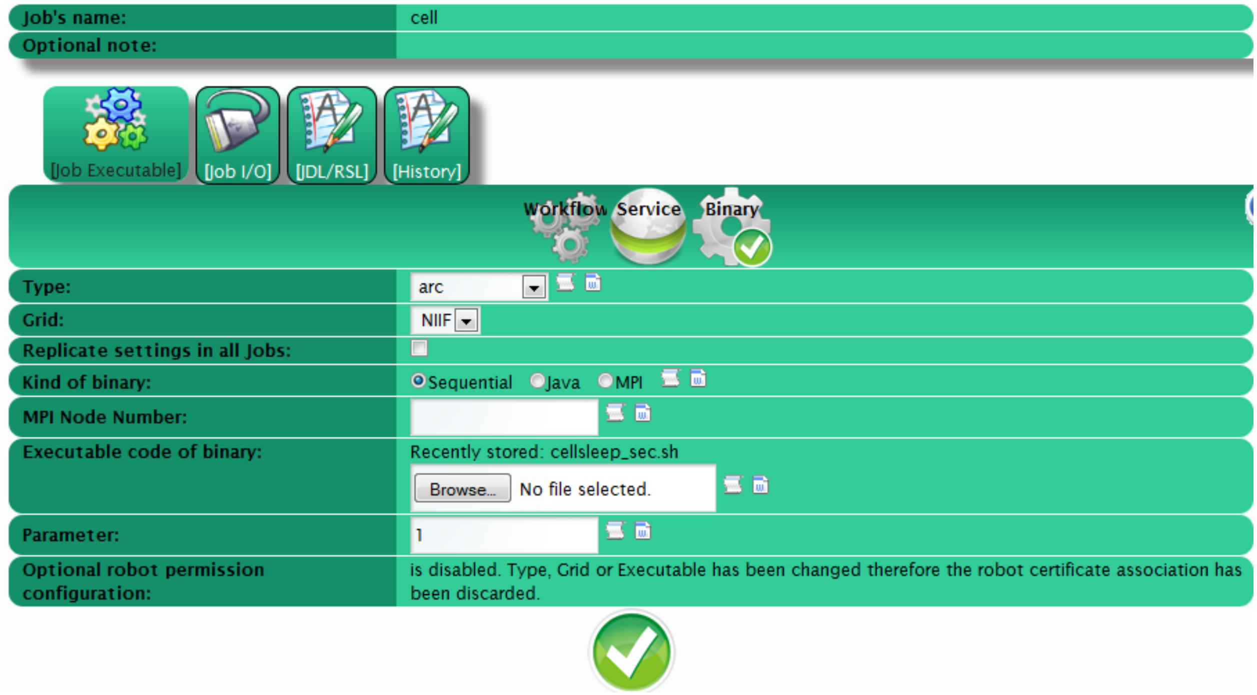
Another option for using executable binary code: using of local browser for uploading executable binary code. The using of this solution is mandatory if no **Preloaded executable** has been defined previously (the field of selected **Preloaded executables** is empty).

Part E The two options of UNICORE-based job configuration: using of Preloaded executables (above) or using of Executable code of binary (below)


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Binary

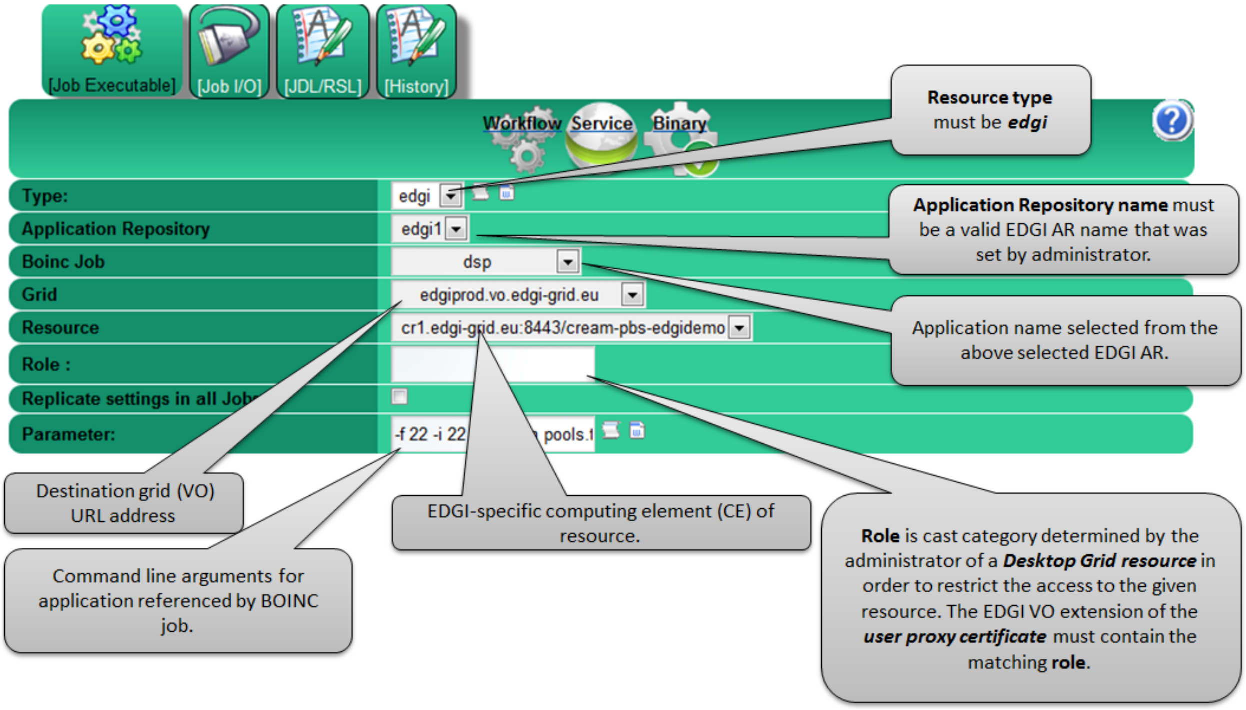
Type:	pbs
Resource:	pbs0.cloud
JobManager:	test
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	● Local ○ Remote Recently stored: sleep_sec.sh Browse... No file selected.
Parameter:	2
Optional robot permission configuration:	is disabled. Type, Grid or Executable is(are) under change. Save the changed job and workflow beforehand.
Assigned breakpoint:	● No breakpoint ○ Before submission ○ After termination Blocker timeout of user interaction: 0

Part F PBS-LFS configuration


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Service
Binary

Job's name:	cell
Optional note:	
Type:	arc
Grid:	NIIF
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	Recently stored: cellsleep_sec.sh Browse... No file selected.
Parameter:	1
Optional robot permission configuration:	is disabled. Type, Grid or Executable has been changed therefore the robot certificate association has been discarded.

Part G ARC configuration



Type: edgi

Application Repository: edgi1

Boinc Job: dsp

Grid: edgiprod.vo.edgi-grid.eu

Resource: cr1.edgi-grid.eu:8443/cream-pbs-edgidemo

Role :

Replicate settings in all Jobs: ☐

Parameter: -f 22 -i 22 … pools.t

Resource type must be ***edgi***

Application Repository name must be a valid EDGI AR name that was set by administrator.

Application name selected from the above selected EDGI AR.

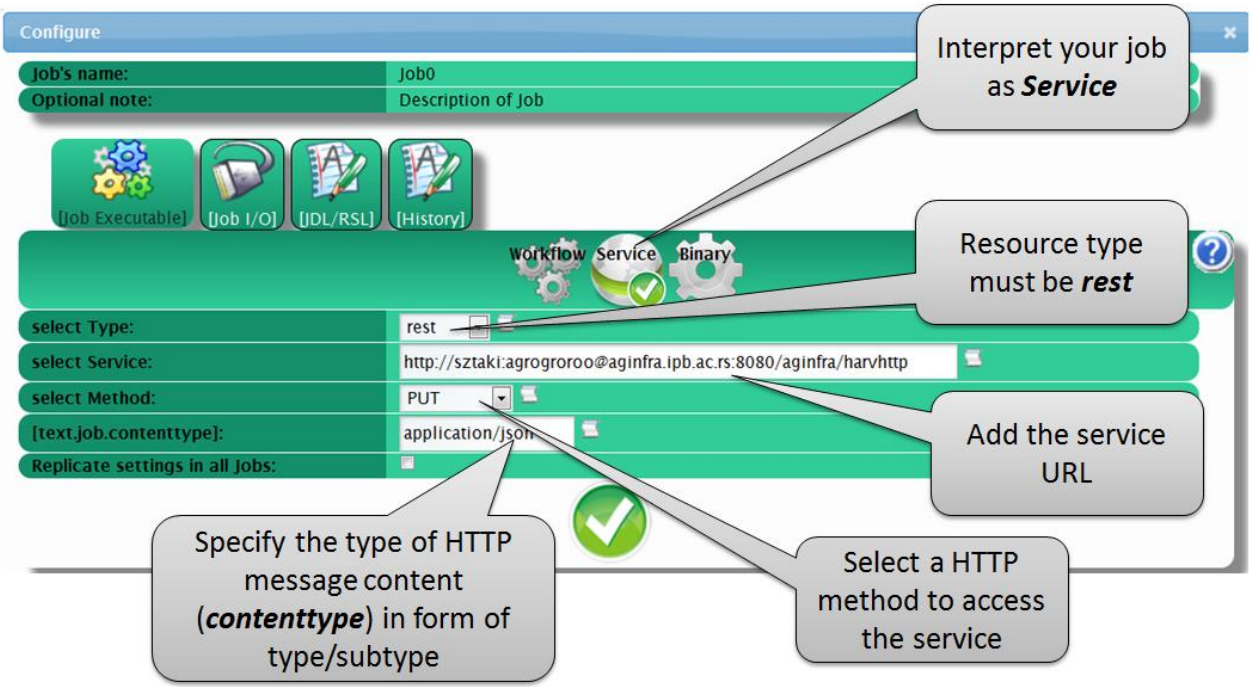
Destination grid (VO) URL address

Command line arguments for application referenced by BOINC job.

EDGI-specific computing element (CE) of resource.

Role is cast category determined by the administrator of a ***Desktop Grid resource*** in order to restrict the access to the given resource. The EDGI VO extension of the ***user proxy certificate*** must contain the matching **role**.

Part H EDGI configuration



Job's name: Job0

Optional note: Description of Job

select Type: rest

select Service: http://sztaki:agrogroroo@aginfra.ipb.ac.rs:8080/aginfra/harvhttp

select Method: PUT

[text.job.contenttype]: application/json

Replicate settings in all Jobs: ☐

Interpret your job as ***Service***

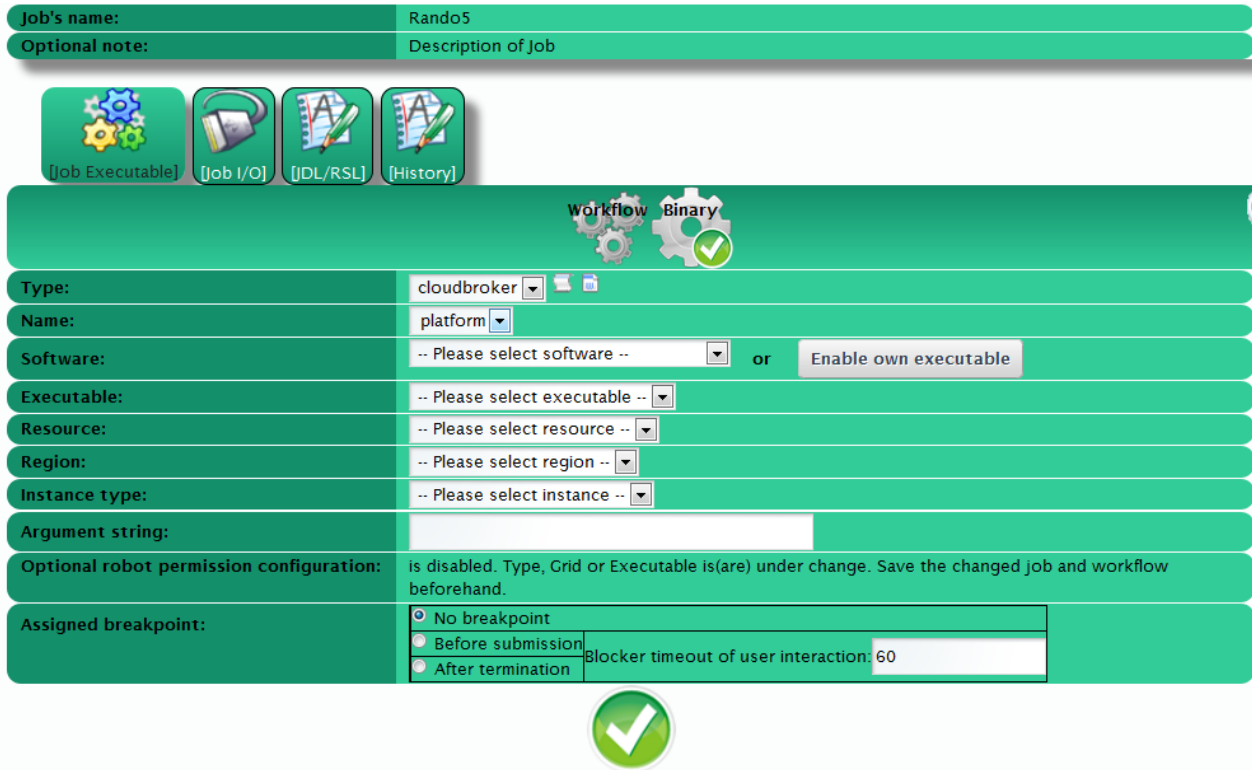
Resource type must be ***rest***

Add the service URL

Specify the type of HTTP message content (***contenttype***) in form of type/subtype

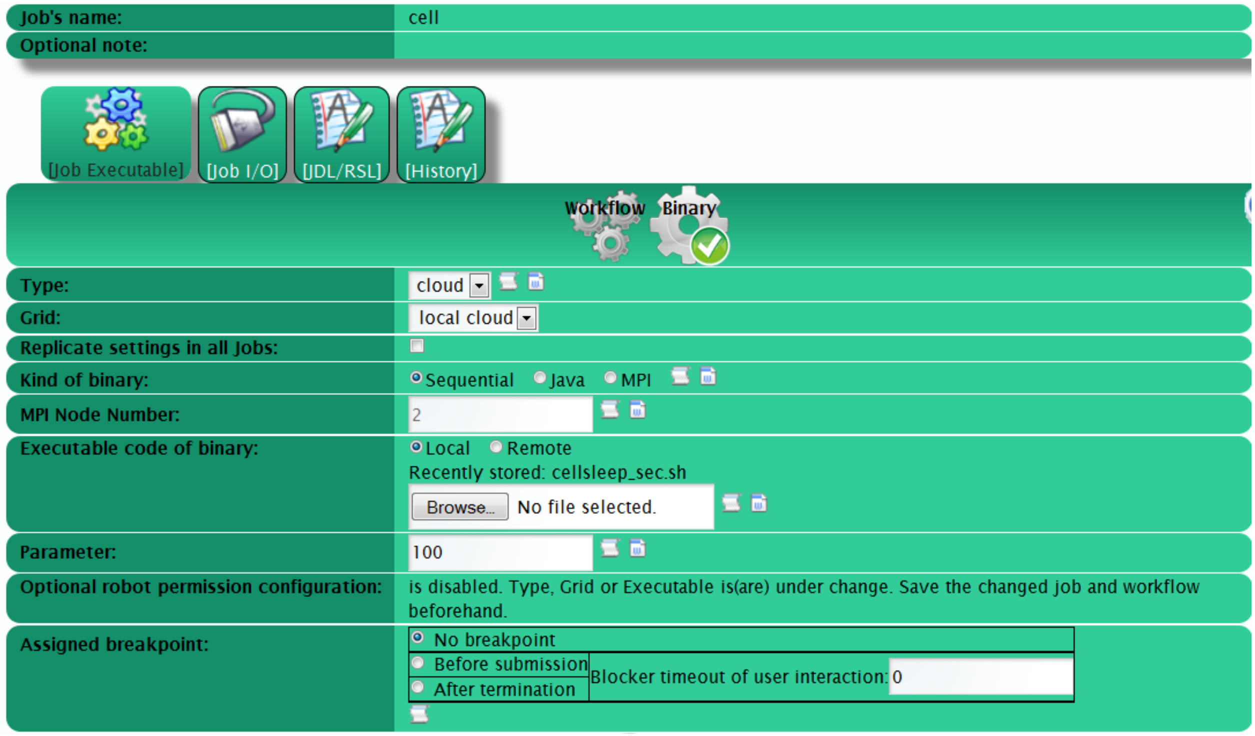
Select a HTTP method to access the service

Part I REST configuration (REST configuration is not differ from GAE and HTTP configuration)


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Binary
Enable own executable

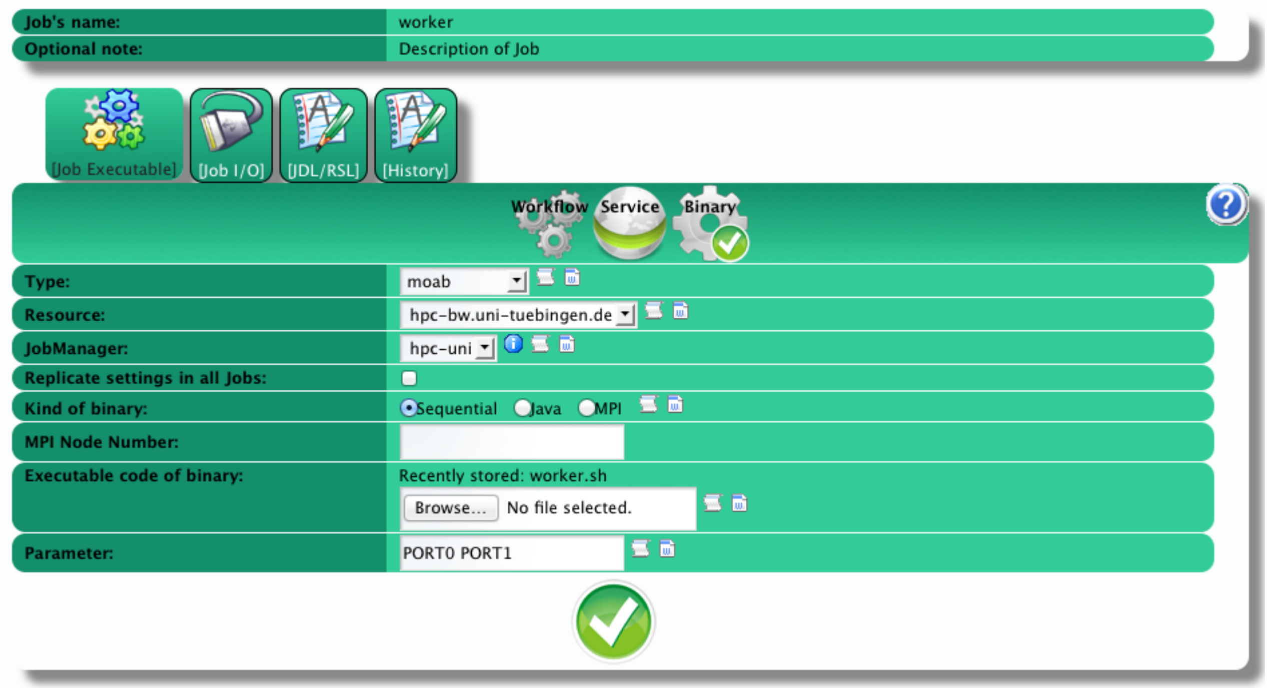
Job's name: Rando5
Optional note: Description of Job
Type: cloudbroker
Name: platform
Software: -- Please select software -- or
Executable: -- Please select executable --
Resource: -- Please select resource --
Region: -- Please select region --
Instance type: -- Please select instance --
Argument string:
Optional robot permission configuration: is disabled. Type, Grid or Executable is(are) under change. Save the changed job and workflow beforehand.
Assigned breakpoint: ● No breakpoint ○ Before submission ○ After termination Blocker timeout of user interaction: 60

Part J CloudBroker configuration


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Binary
Browse...

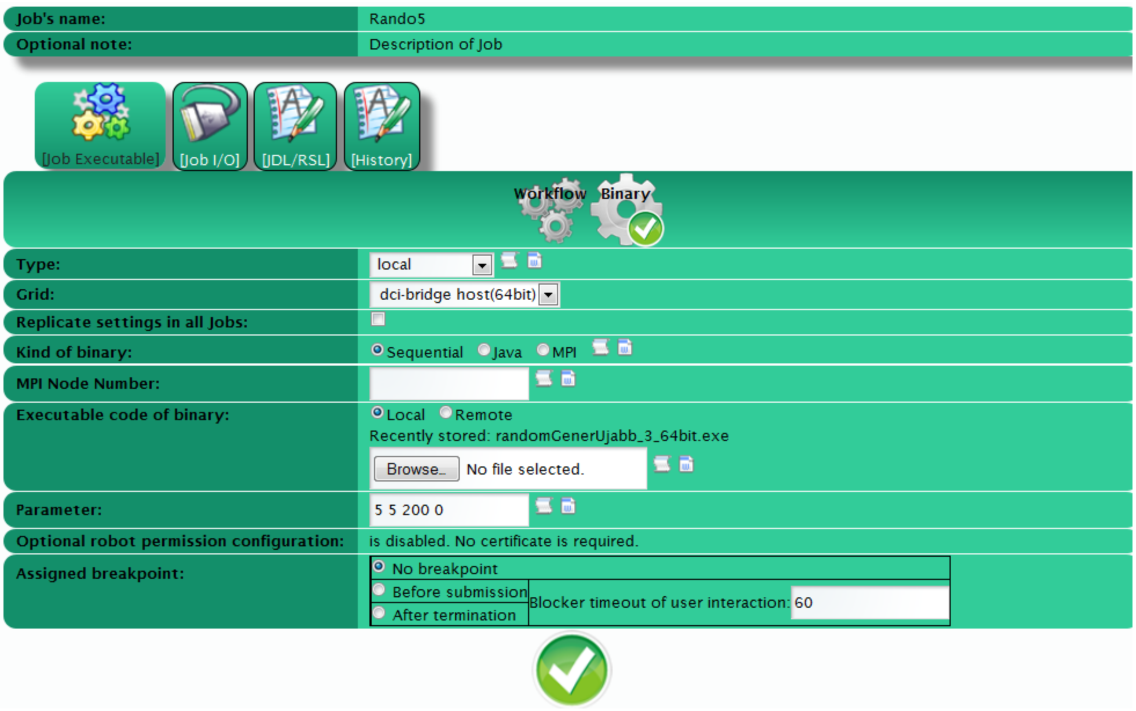
Job's name: cell
Optional note:
Type: cloud
Grid: local cloud
Replicate settings in all Jobs: ☐
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number: 2
Executable code of binary: ● Local ○ Remote
Recently stored: cellsleep_sec.sh
No file selected.
Parameter: 100
Optional robot permission configuration: is disabled. Type, Grid or Executable is(are) under change. Save the changed job and workflow beforehand.
Assigned breakpoint: ● No breakpoint ○ Before submission ○ After termination Blocker timeout of user interaction: 0

Part K Cloud (EC2-based Cloud) configuration



Job's name: worker
Optional note: Description of Job
Type: moab
Resource: hpc-bw.uni-tuebingen.de
JobManager: hpc-uni
Replicate settings in all Jobs: ☐
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: Recently stored: worker.sh
Browse... No file selected.
Parameter: PORT0 PORT1

Part L MOAB[4] configuration



Job's name: Rando5
Optional note: Description of Job
Type: local
Grid: dci-bridge host(64bit)
Replicate settings in all Jobs: ☐
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: ● Local ○ Remote
Recently stored: randomGenerUjabb_3_64bit.exe
Browse... No file selected.
Parameter: 5 5 200 0
Optional robot permission configuration: is disabled. No certificate is required.
Assigned breakpoint: ● No breakpoint
○ Before submission
○ After termination
Blocker timeout of user interaction: 60

Part M Local configuration

Appendix Figure 13 (Part A - Part M) Concrete menu/Configure Job Executable for different middlewares

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[4] The MOAB plugin development comes from the gUSE Community (exactly from Applied Bioinfomatics Group of Eberhard Karls University, Tübingen). If you have further questions, please send it to Luis de la Garza (delagarza@informatik.uni-tuebingen.de).

The main window ofjob configuration contains four selectable sub tabs:

- ***Job Executable***
- ***Job I/O***
- ***JDL-RSL***
- ***History***

The default active one Job Executable has distinguished importance and its setting determines whether the tabs Job I/O and JDL-RSL have meaning at all. Job Executable determines:

- the basic type of algorithm (embedded workflow invocation, service call, binary code, Cloud based execution);
- the way the algorithm is associated to an executing resources (in the case of binary code);
- the algorithm itself.

There may be a difference whether the algorithm is supplied by the user in form of an uploaded code file or it is only selectable from a list offered online by a remote resource (when the base algorithm is service call or when the *Type* of the resource is *SHIWA*).

In both cases control parameters can be associated to the algorithm. The fields of the form in case of binary code may be grouped in the following categories showed depending on the kind of the selected Type: *Type, Grid, Resource, JobManager* determines the destination where the job will be executed.

The fields *Kind of binary, MPI Node Number, Executable code of binary, Parameter* define the code of the algorithm to be uploaded. These settings must be confirmed by clicking on the *Save* button.

Note: Please remember that saving the job does not ensure the saving/updating of the workflow in itself: the user must hit the *Save on Server* button in the "parent window" before leaving the workflow configuration.

Special considerations about embedding of workflow: the insulated computational logic hidden behind of a single job may be the invocation of an existing defined workflow of the same user. As the input ports of the caller jobs may be associated to certain genuine input ports of the called (embedded) workflow and certain output ports of the called (embedded) workflow can be associated to the output ports of the caller job, the mode of evaluation corresponds to the classical subroutine call paradigm.

Moreover the call can be - explicitly or implicitly - a recursive one as a new workflow instance object will be created upon the submission of a workflow (storing the intermediate files encoding the run time state and the output files of the workflow).

With the common application of the input condition (on job ports) and with the application of the recursive embedding the DAG imposed ban on the repeated call of a job of the workflow can be circumvented. The other trivial way of bypassing is the PS. However in the current implementation there are rather strong restrictions when the embedded workflow call can be used:

An embedded workflow, within a PS environment - knowing nothing about the number of its proposed invocation – cannot be used. The main cause is that the index space of the PS regime is calculated –for the time being – in a static way, before the invocation of the workflow.

On the input side only the passing of the local (uploaded or channel) files are supported, but there is no support for remote files, or of unnamed files built of direct values which may be defined during port configuration at common input ports.

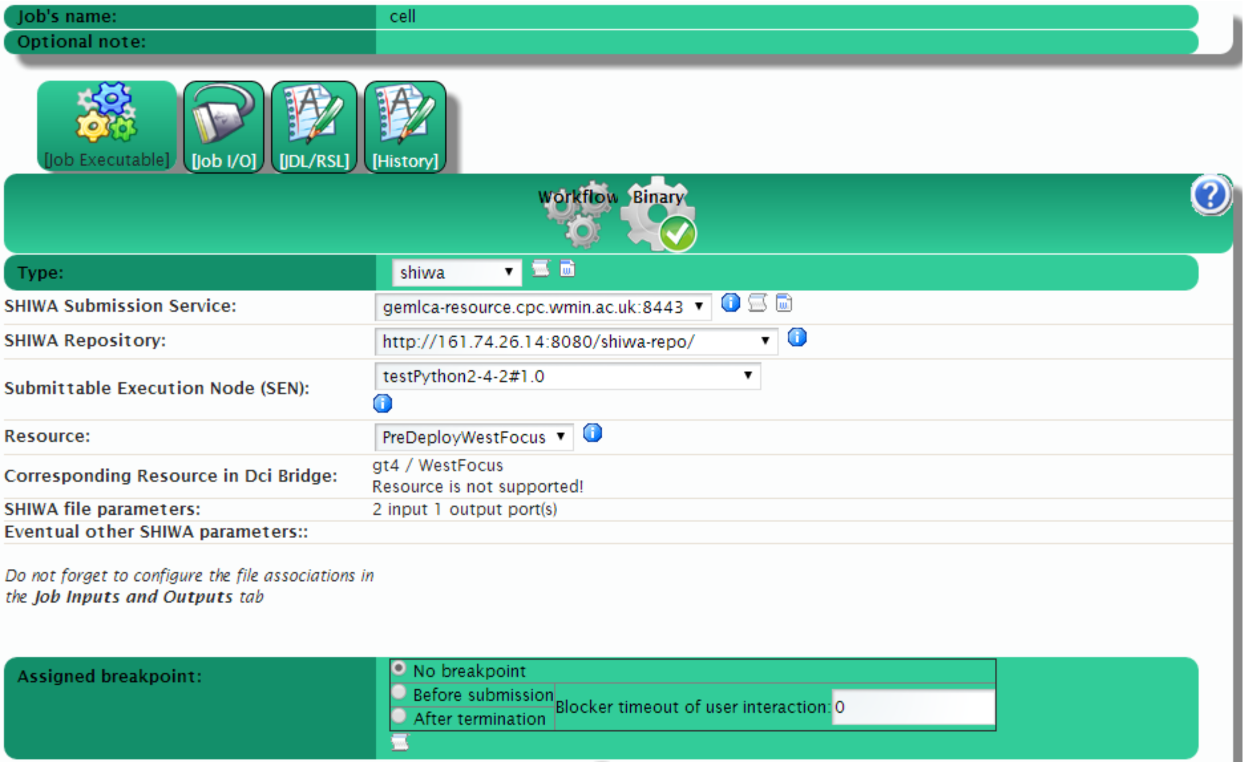
Neither can be used the SQL input – which would combine the difficulties mentioned at the PS and the direct value cases.

On the output side the local file generated by the embedded workflow cannot be associated to a remote file defined on the output port of the caller job.

Neither the ports of the embedded workflow associated to a remote file are may not be involved in parameter passing.

Technically the configuration of embedded workflow call happens in two steps:

In the *Job Executable* tab (*Workflow/Concrete* tab -> selected workflow -> selected job) the choice "*Interpretation of job as Workflow*" will be selected as job execution model, and from the list labeled as "for embedding select a workflow created from a template:" a proper workflow will be selected. In the parallel *Job Inputs and Outputs* tab there is the option "Connect input port to a Job/Input port of the embedded WF" to each input port of the caller job. If the option is selected then the list of associable input ports of the embedded workflow will be selectable sowed as job/port name pair. Similar is true for the output ports selecting the "*Connect output port to a Job/Output port of the embedded WF*" option.



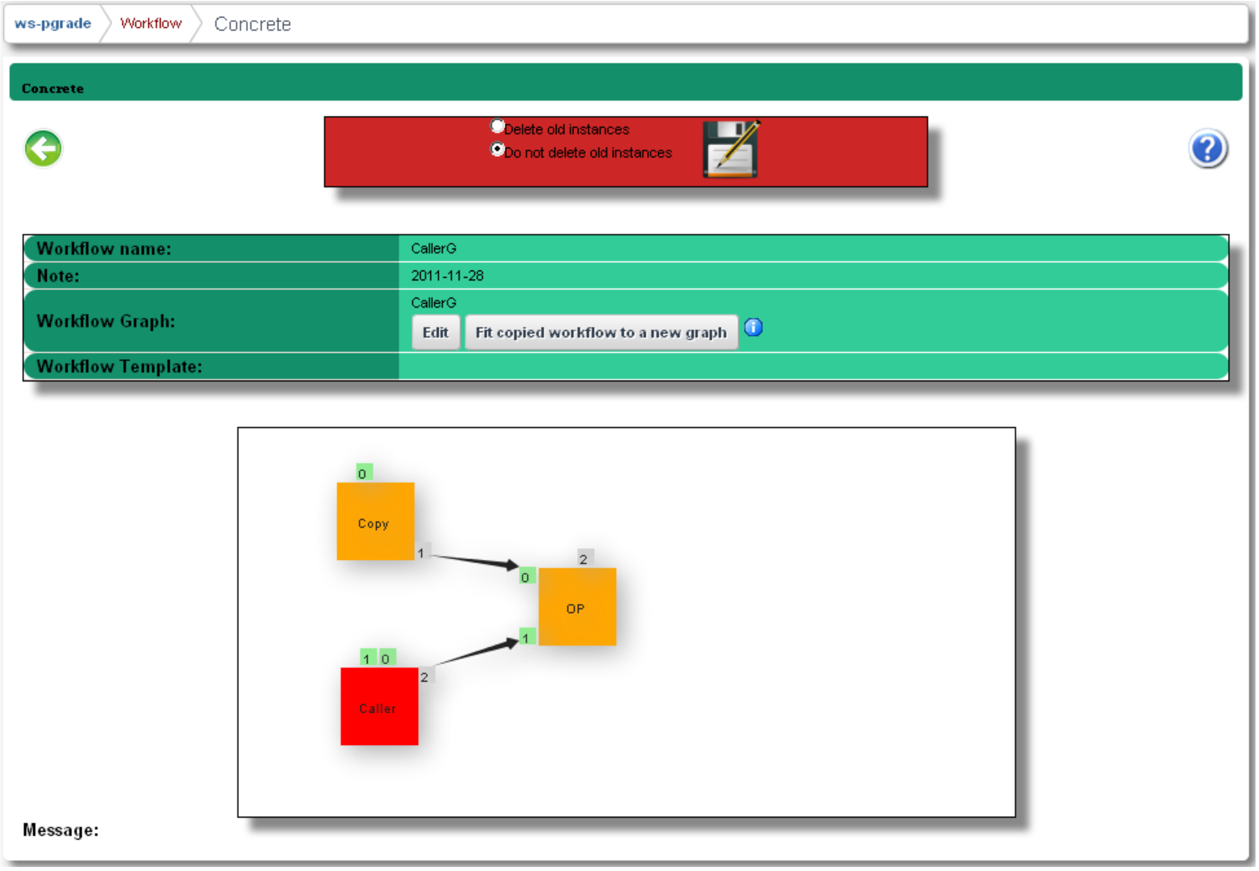
Job's name: cell
Optional note:

Type: shiwa
SHIWA Submission Service: gemlca-resource.cpc.wmin.ac.uk:8443
SHIWA Repository: http://161.74.26.14:8080/shiwa-repo/
Submittable Execution Node (SEN): testPython2-4-2#1.0
Resource: PreDeployWestFocus
Corresponding Resource in Dci Bridge: gt4 / WestFocus
Resource is not supported!
SHIWA file parameters: 2 input 1 output port(s)
Eventual other SHIWA parameters::

*Do not forget to configure the file associations in the **Job Inputs and Outputs** tab*

Assigned breakpoint:
● No breakpoint
○ Before submission
○ After termination
Blocker timeout of user interaction: 0

Appendix Figure 14 Concrete menu, Configure Job Executable, when Type is SHIWA after Repository Selection

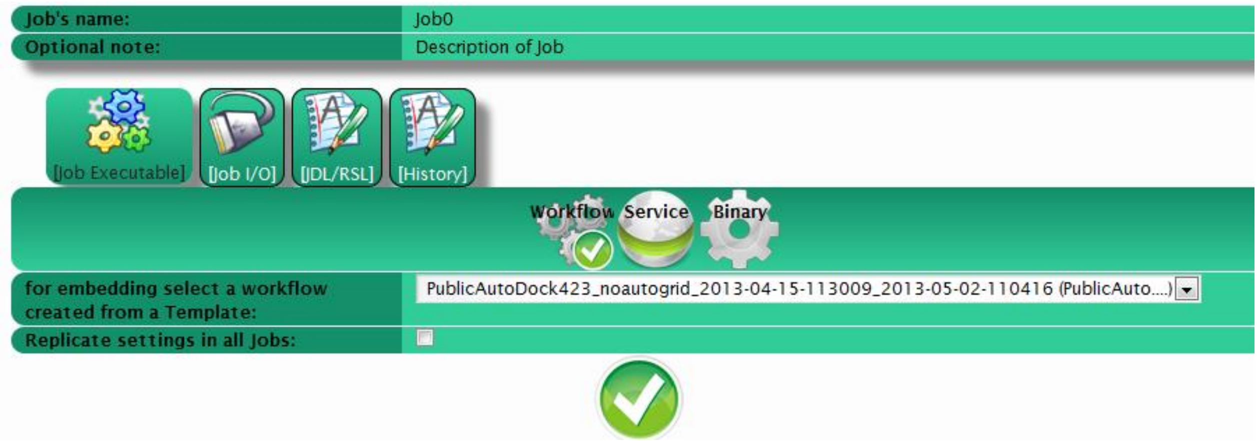

ws-pgrade
Workflow
Concrete
Concrete
Copy
OP
Caller
0
1
2
0
1
1 0
2

○ Delete old instances
● Do not delete old instances

Workflow name:	CallerG
Note:	2011-11-28
Workflow Graph:	CallerG Edit Fit copied workflow to a new graph
Workflow Template:	

Message:

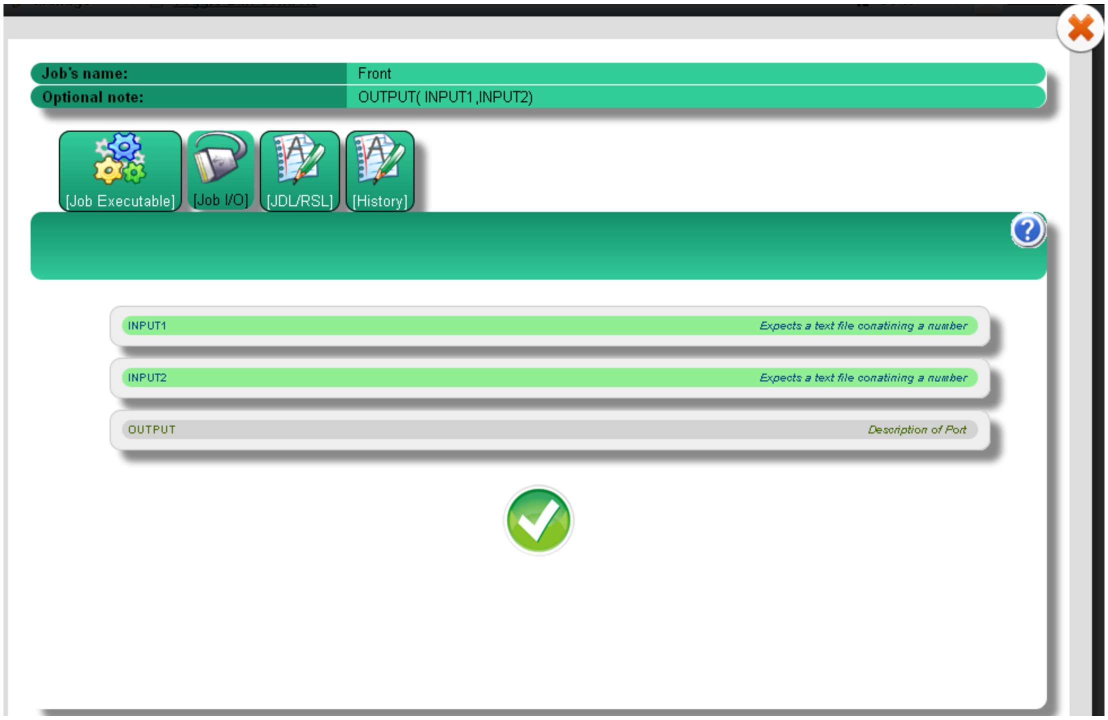
Appendix Figure 16a Concrete menu, Configure Workflow calling Job - select job


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Service
Binary

Job's name:	Job0
Optional note:	Description of Job
for embedding select a workflow created from a Template:	PublicAutoDock423_noautogrid_2013-04-15-113009_2013-05-02-110416 (PublicAuto....)
Replicate settings in all Jobs:	☐

Appendix Figure 16b Concrete menu, Configure Workflow calling Job - configure embedded

3.2.2 The Concrete/Configure/Job Inputs and Outputs Tab



Job's name: Front

Optional note: OUTPUT(INPUT1 ,INPUT2)

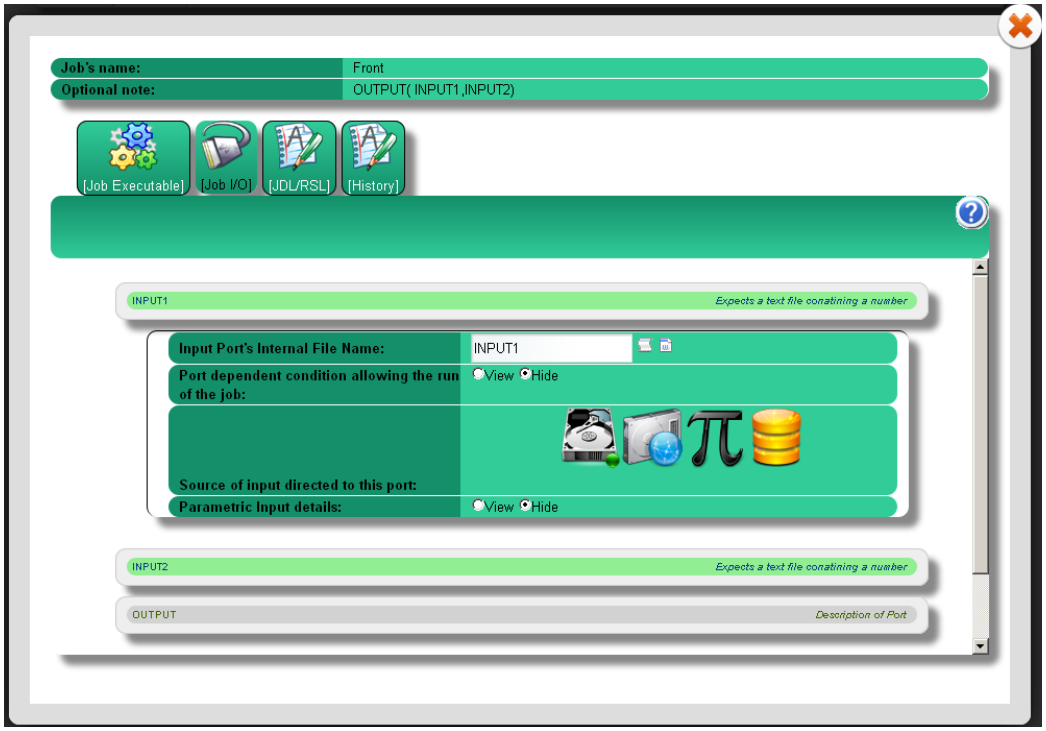
INPUT1 — Expects a text file conatining a number

INPUT2 — Expects a text file conatining a number

OUTPUT — Description of Port

Appendix Figure 17a Job Inputs and Outputs Tab, Main View

Clicking on any of the input or output ports opens the detailed mode: please note that the actual appearance is dependent on the context and history of the Port.



Job's name: Front

Optional note: OUTPUT(INPUT1 ,INPUT2)

INPUT1 — Expects a text file conatining a number

Input Port's Internal File Name: INPUT1

Port dependent condition allowing the run of the job: ○View ●Hide

Source of input directed to this port:

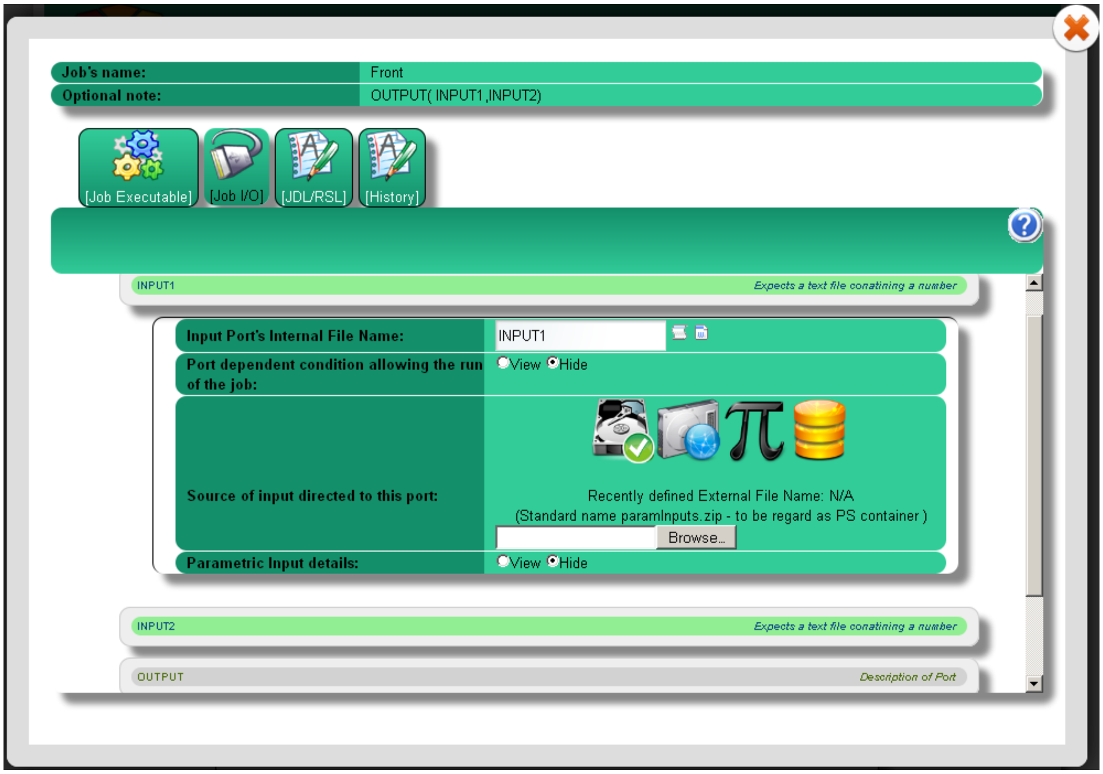
Parametric Input details: ○View ●Hide

INPUT2 — Expects a text file conatining a number

OUTPUT — Description of Port

Appendix Figure 17b Input Port with no previous configuration

If there has been no previous configuration, and the input port is not the destination (end point) of a channel then an icon must be selected of the group source of input directed to this port:



Job's name: Front
Optional note: OUTPUT(INPUT1,INPUT2)

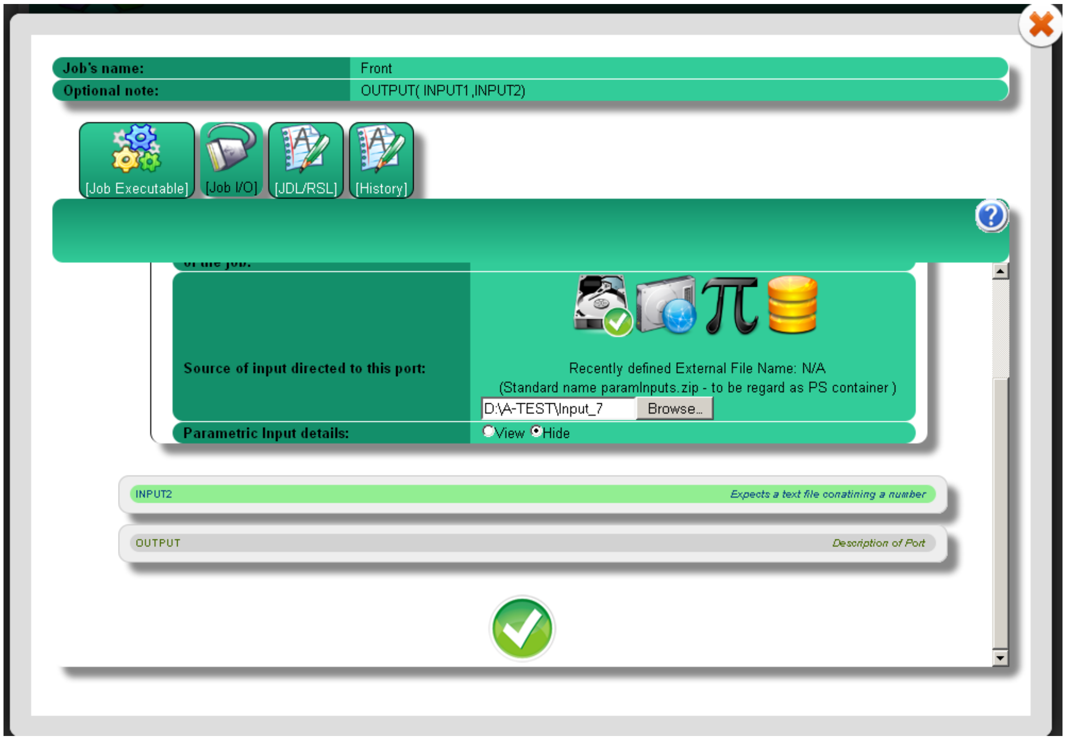
INPUT1 — *Expects a text file conatining a number*

Input Port's Internal File Name: INPUT1
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port: Recently defined External File Name: N/A (Standard name paramInputs.zip - to be regard as PS container)
Parametric Input details: ○View ●Hide

INPUT2 — *Expects a text file conatining a number*

OUTPUT — *Description of Port*

Appendix Figure 17c Concrete Configure Ports: Selected Source of input is File Upload



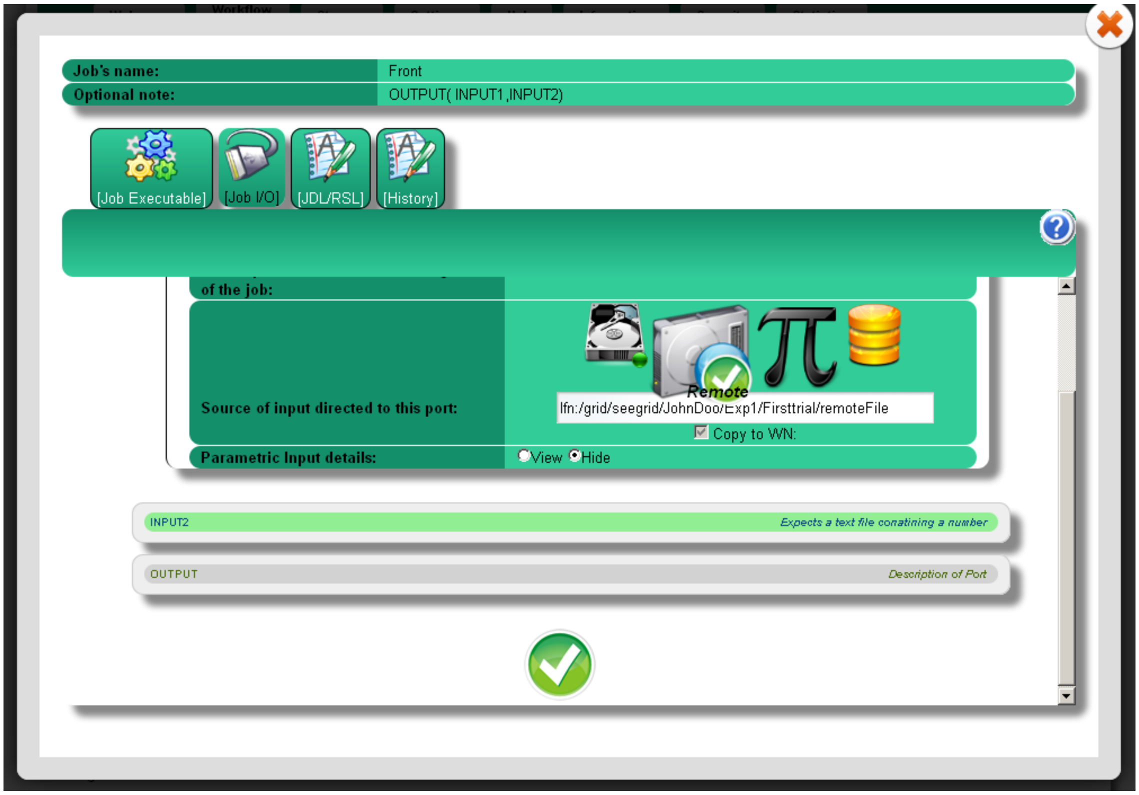
Job's name: Front
Optional note: OUTPUT(INPUT1,INPUT2)

Source of input directed to this port: Recently defined External File Name: N/A (Standard name paramInputs.zip - to be regard as PS container) D:\A-TEST\Input_7
Parametric Input details: ○View ●Hide

INPUT2 — *Expects a text file conatining a number*

OUTPUT — *Description of Port*

Appendix Figure 18a Concrete Configure Ports to the selected Job – after configuring a File Upload

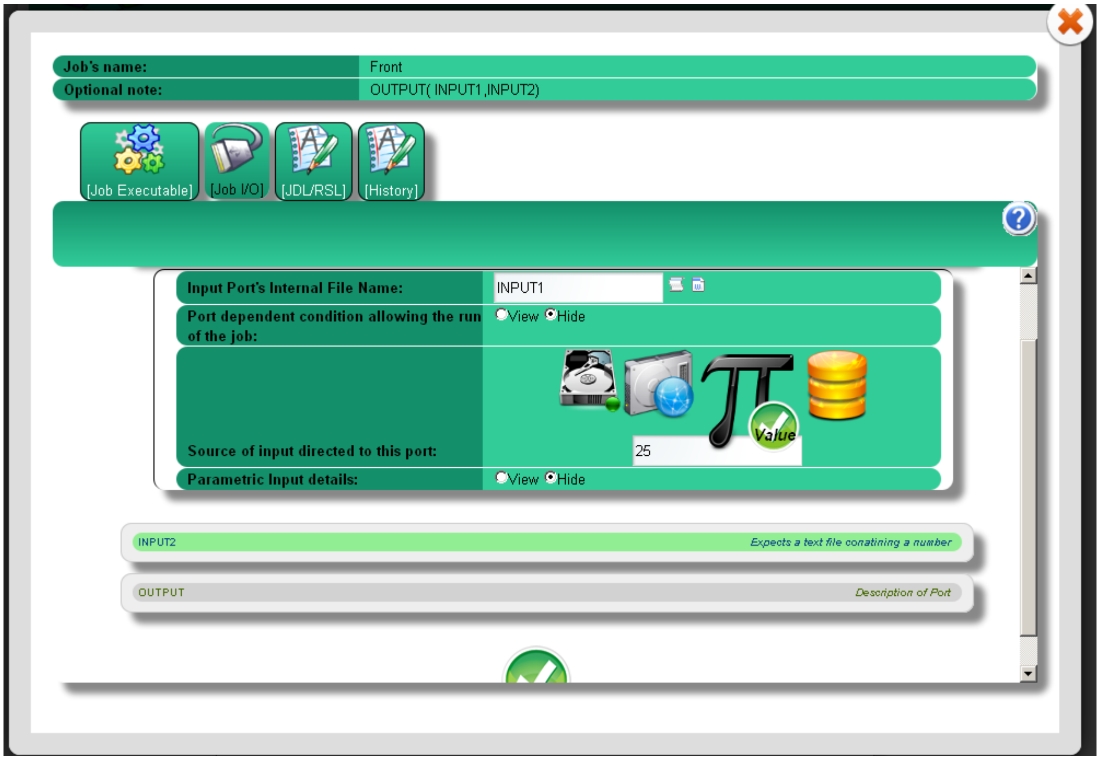


Job's name: Front
Optional note: OUTPUT(INPUT1 ,INPUT2)

of the job:
Source of input directed to this port: lfn:/grid/seegrid/JohnDoo/Exp1/Firsttrial/remoteFile
☑ Copy to WN:
Parametric Input details: ○View ●Hide

INPUT2 Expects a text file conatining a number
OUTPUT Description of Port

Appendix Figure 18b Concrete Configure Ports to the selected Job – after configuring a Remote file reference

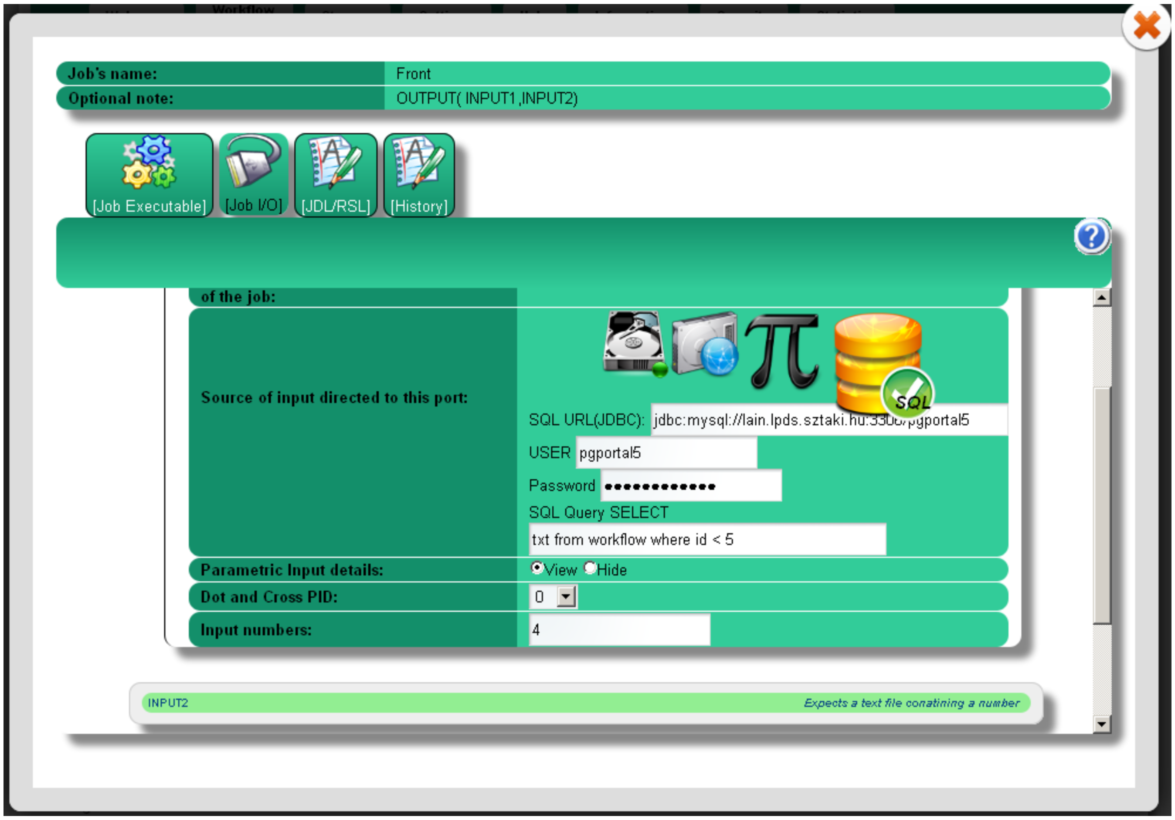


Job's name: Front
Optional note: OUTPUT(INPUT1 ,INPUT2)

Input Port's Internal File Name: INPUT1
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port: 25
Parametric Input details: ○View ●Hide

INPUT2 Expects a text file conatining a number
OUTPUT Description of Port

Appendix Figure 18c Concrete Configure Ports to the selected Job – after configuring a constant value



Job's name: Front
Optional note: OUTPUT(INPUT1,INPUT2)

of the job:
Source of input directed to this port:
SQL URL(JDBC): jdbc:mysql://lain.lpds.sztaki.hu:3306/pgportal5
USER pgportal5
Password •••••••••••••
SQL Query SELECT
txt from workflow where id < 5
Parametric Input details: ● View ○ Hide
Dot and Cross PID: 0
Input numbers: 4

INPUT2 *Expects a text file conatining a number*

Appendix Figure 18d Concrete Configure Ports to the selected Job – after configuring an SQL query

This form lists the ports belonging to the actual job with the proper configuration possibilities. Please notice the inner vertical ruler to select the port to be configured. The ports subdivided in two lists: First the input ports, after the output ports are encountered.

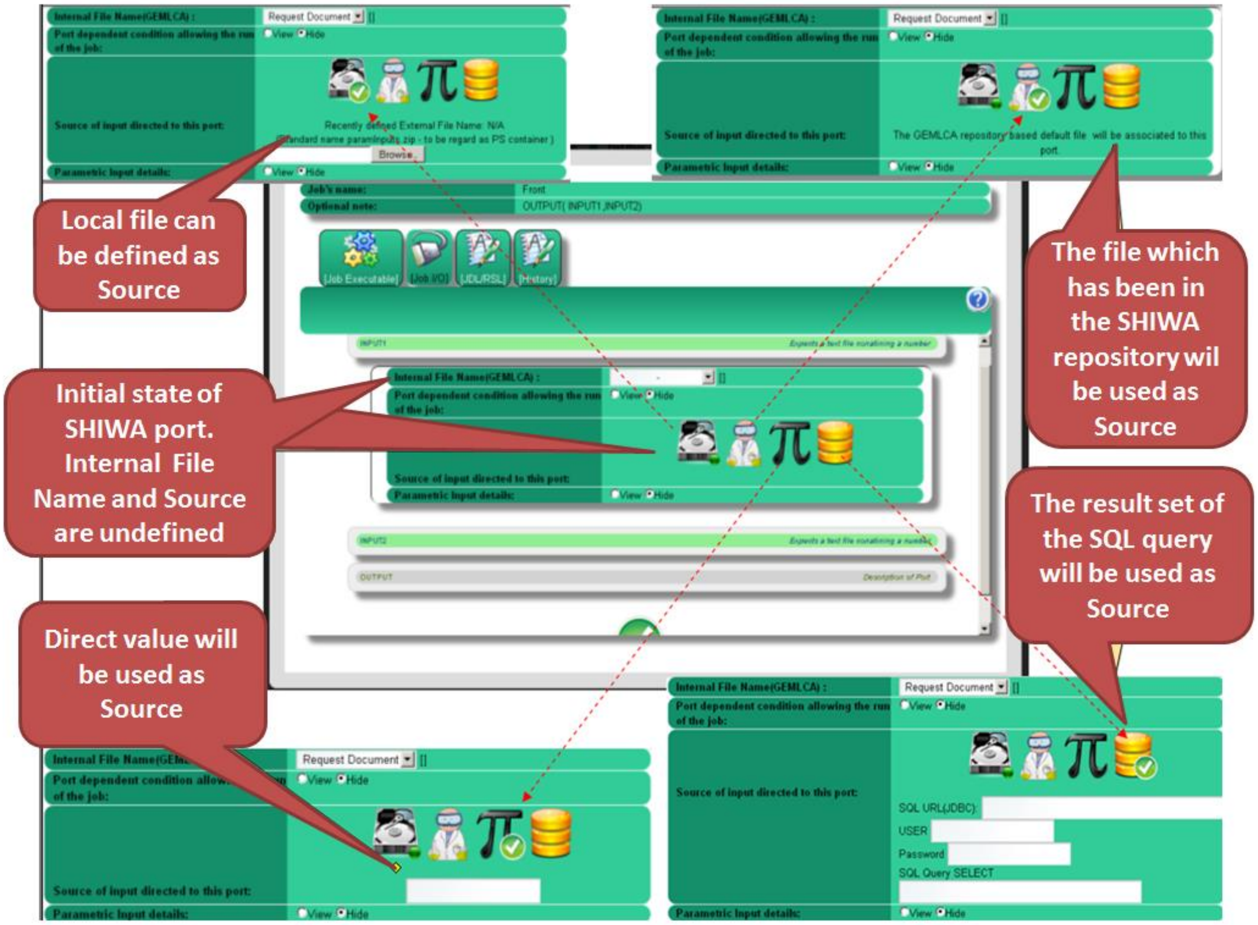
Each port inherits the port name from the graph description as the default value for the internal file name. As the uploaded executable code references the proper Internal File Name in order to open an input or an output file, its value must be known - and set - by the user to configure the connection properly. In several other respects the configuration of input and output ports may be different. In case of input ports:

- There is a possibility to define a condition about the content of the file in order to permit/refuse the execution of the associated job.
- There is a wide palette (Upload (see Figure 18a), *Remote* (see Figure 18b), *Value* (see Figure 18/c), *SQL* (see Figure 18d) to define the external source/content of the values to be forwarded through the given input port. Note, that the port in this case must not be the endpoint of a channel (statically associated to the output port of a job of the same workflow by the graph description)
- There is an option (*Parametric Input details*) to define a multiplication factor for job submissions and to relate the input sets forwarded through this port to other sibling ports of the same job.

The handling of input ports in case of SHIWA jobs is slightly different: The *Internal File Names* must be selected from the set supplied by the SHIWA Repository and they should be associated to the ports explicitly. See Appendix Figure 19.

Warning: In the new user interface there is no default selection for the *Source of input directed to this port*. It must be defined! In case of output ports: there is an optional entry to define the destination if the respective output stream of the job is directed to a remote file. There is the *Generator* value 1 which can be modified in case of parameter sweep when the job is instructed to produce the required number of output files through this port in order to trigger the proper number of invocations of the subsequent connected jobs. A special optional entry appears for each port if the user has defined the current job to call an embedded workflow in the *Job Executable* tab i.e. the radio button value *Interpretation of job as workflow has been selected*. This entry is labeled as *Connect to embedded WF's port* posing the current port as "formal parameter" to which the proper port of the called (embedded) workflow as *actual parameter* can be associated. The association ensures the automatic file transfers before/after the execution of the embedded workflow respectively.

Note: the association is not obligatory in the input port case: There may be a defined input value having been associated to the proper port of the embedded workflow. These settings must be confirmed by clicking on the button OK. Please, remember that saving the port settings of the job does not ensure the saving/updating of the workflow in itself.



Internal File Name(GEMLCA) : Request Document []
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port: Recently defined External File Name: N/A (Standard name paramInputs.zip - to be regard as PS container)
Parametric Input details: ○View ●Hide

Local file can be defined as Source

Internal File Name(GEMLCA) : Request Document []
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port: The GEMLCA repository based default file will be associated to this port.
Parametric Input details: ○View ●Hide

The file which has been in the SHIWA repository wil be used as Source

Job's name: Front
Optional note: OUTPUT(INPUT1,INPUT2)

Initial state of SHIWA port. Internal File Name and Source are undefined

Internal File Name(GEMLCA) : - []
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port:
Parametric Input details: ○View ●Hide

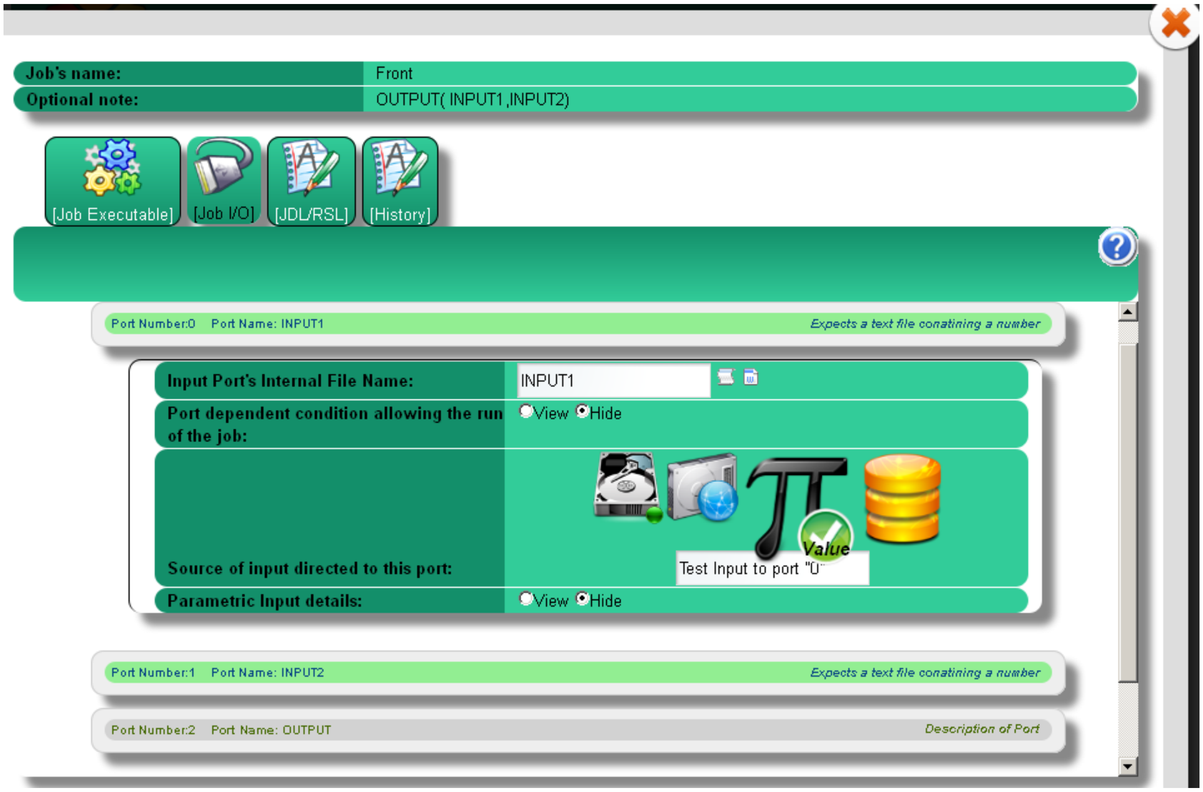
The result set of the SQL query will be used as Source

Direct value will be used as Source

Internal File Name(GEMLCA) : Request Document []
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port:
Parametric Input details: ○View ●Hide

Internal File Name(GEMLCA) : Request Document []
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port: SQL URL(JDBC): USER Password SQL Query SELECT
Parametric Input details: ○View ●Hide

Appendix Figure 19 Input port configuration possibilities in case of SHIWA - note the DEFAULT mode


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Value

Job's name: Front
Optional note: OUTPUT(INPUT1,INPUT2)

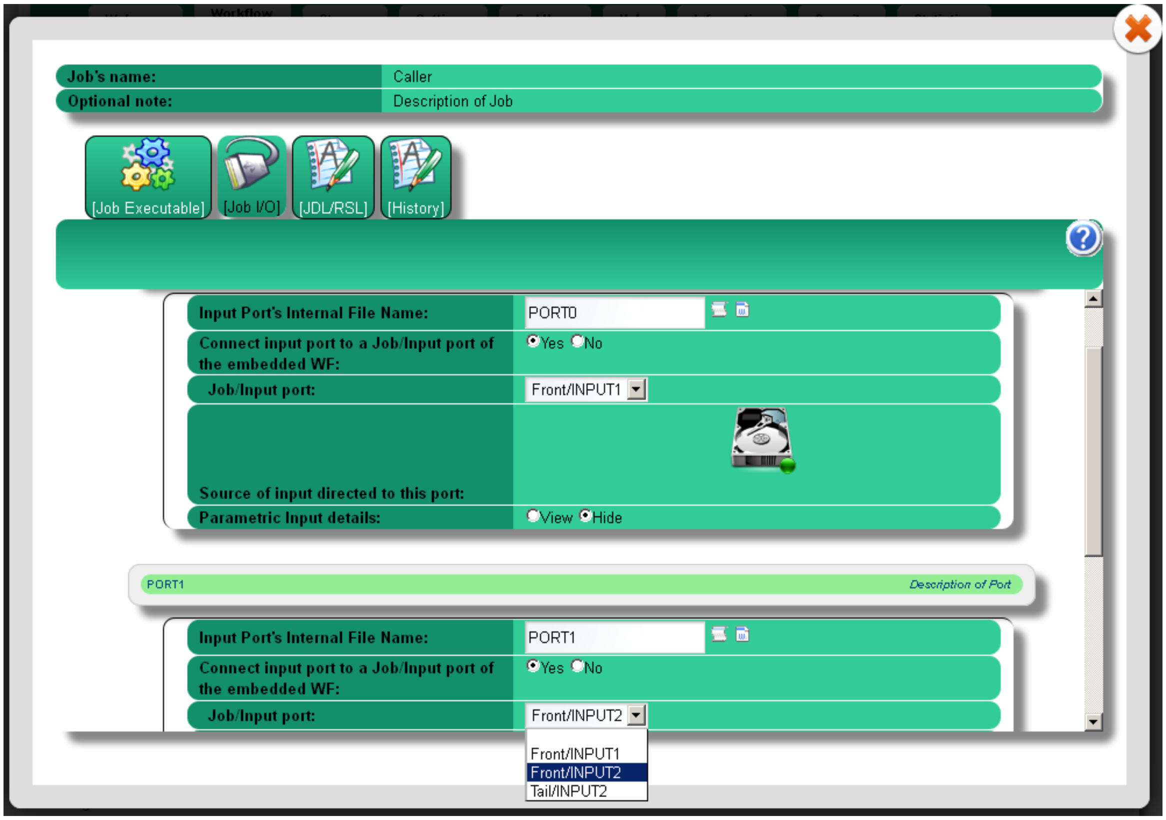
Port Number:0 Port Name: INPUT1 *Expects a text file conatining a number*

Input Port's Internal File Name: INPUT1
Port dependent condition allowing the run of the job: ○View ●Hide
Source of input directed to this port: Test Input to port "0"
Parametric Input details: ○View ●Hide

Port Number:1 Port Name: INPUT2 *Expects a text file conatining a number*

Port Number:2 Port Name: OUTPUT *Description of Port*

Appendix Figure 20 Configuring Port "0" to the selected Service call Job


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Front/INPUT1
Front/INPUT2
Tail/INPUT2

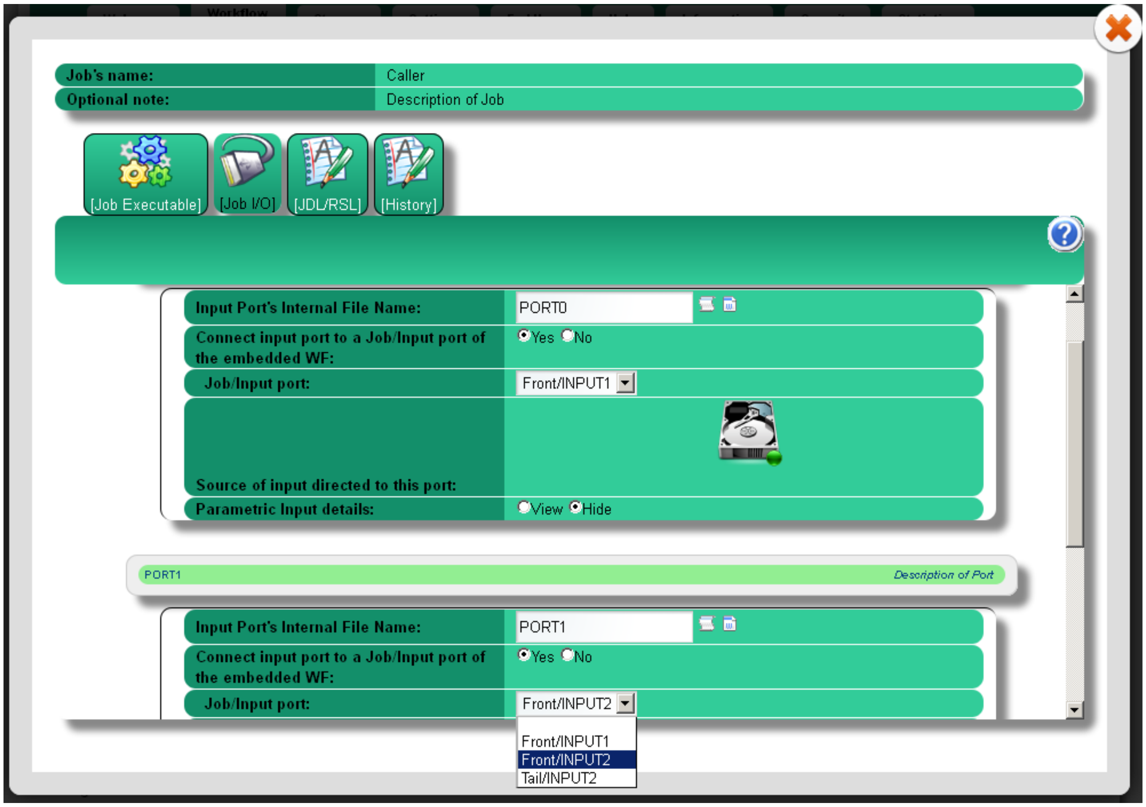
Job's name: Caller
Optional note: Description of Job

Input Port's Internal File Name: PORT0
Connect input port to a Job/Input port of the embedded WF: ●Yes ○No
Job/Input port: Front/INPUT1
Source of input directed to this port:
Parametric Input details: ○View ●Hide

PORT1 *Description of Port*

Input Port's Internal File Name: PORT1
Connect input port to a Job/Input port of the embedded WF: ●Yes ○No
Job/Input port: Front/INPUT2

Appendix Figure 21 Concrete Configure Ports to the call of the Selected Workflow


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]

Job's name: Caller
Optional note: Description of Job

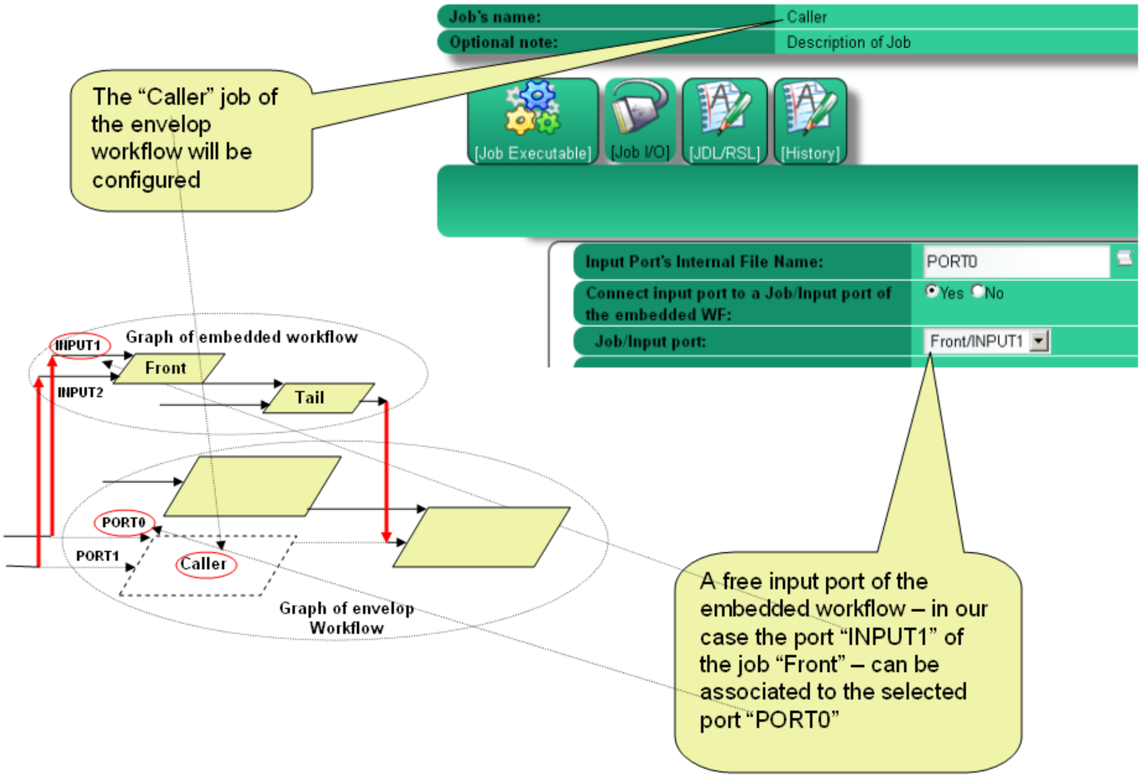
Input Port's Internal File Name: PORT0
Connect input port to a Job/Input port of the embedded WF: ● Yes ○ No
Job/Input port: Front/INPUT1
Source of input directed to this port:
Parametric Input details: ○ View ● Hide

PORT1 *Description of Port*

Input Port's Internal File Name: PORT1
Connect input port to a Job/Input port of the embedded WF: ● Yes ○ No
Job/Input port: Front/INPUT2

Front/INPUT1
Front/INPUT2
Tail/INPUT2

Appendix Figure 22 Explanation to Figure 21


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Graph of embedded workflow
INPUT1
INPUT2
Front
Tail
PORT0
PORT1
Caller
Graph of envelop Workflow

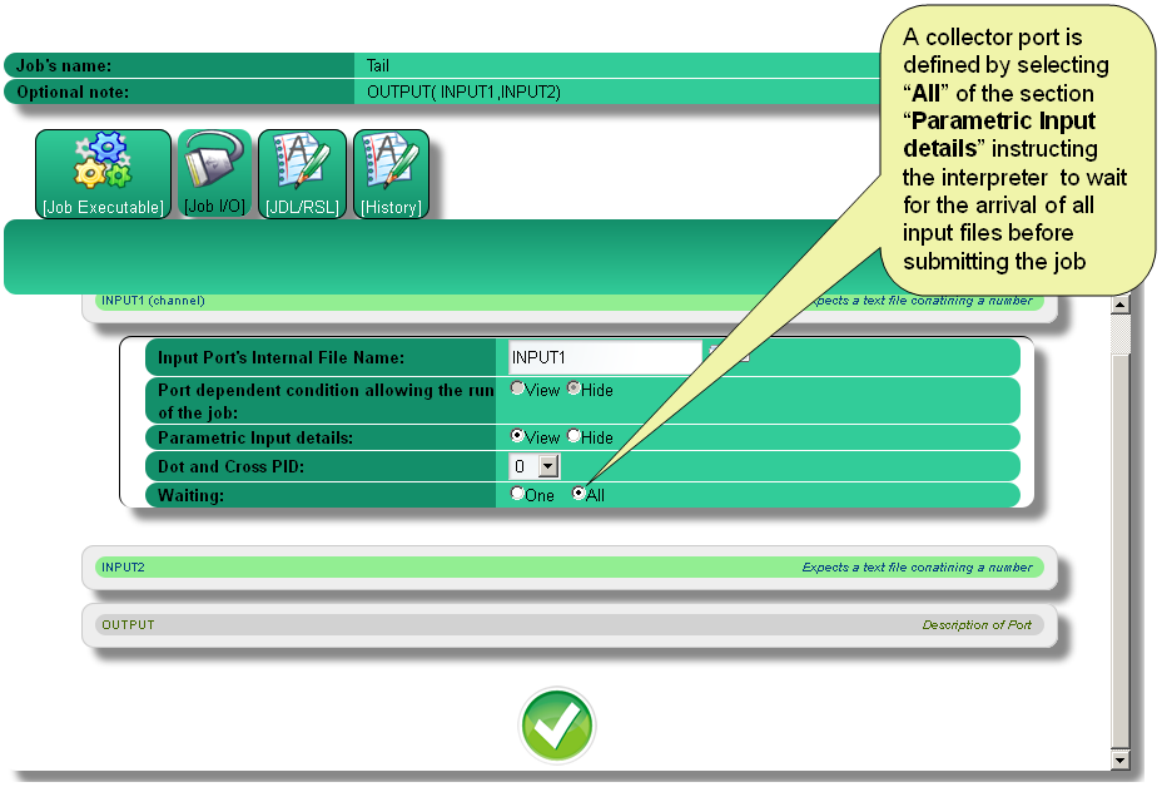
Job's name: Caller
Optional note: Description of Job

Input Port's Internal File Name: PORT0
Connect input port to a Job/Input port of the embedded WF: ● Yes ○ No
Job/Input port: Front/INPUT1

The "Caller" job of the envelop workflow will be configured

A free input port of the embedded workflow – in our case the port "INPUT1" of the job "Front" – can be associated to the selected port "PORT0"

Appendix Figure 23 Configuring Condition to Port permitting run of Job

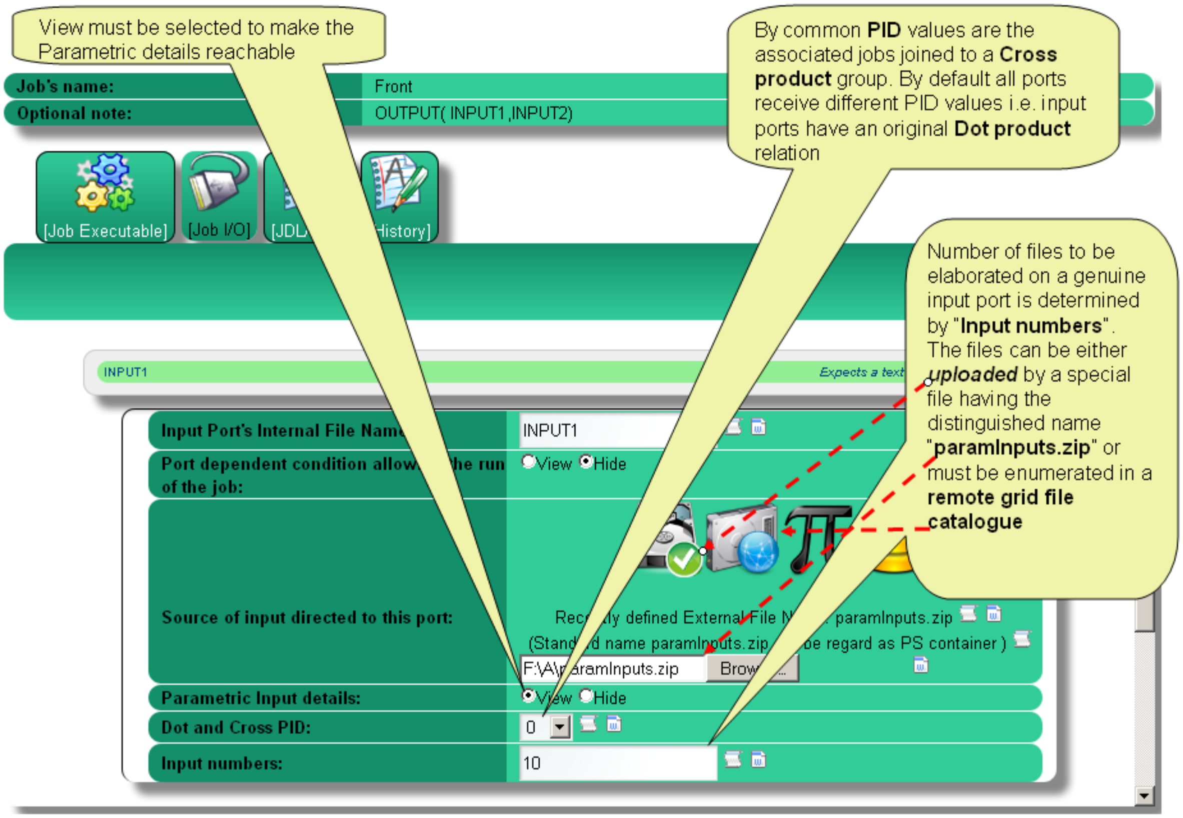

[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
INPUT1 (channel)
Expects a text file conatining a number
INPUT2
Expects a text file conatining a number
OUTPUT
Description of Port

Job's name: Tail
Optional note: OUTPUT(INPUT1,INPUT2)

Input Port's Internal File Name: INPUT1
Port dependent condition allowing the run of the job: ○View ●Hide
Parametric Input details: ●View ○Hide
Dot and Cross PID: 0
Waiting: ○One ●All

A collector port is defined by selecting "**All**" of the section "**Parametric Input details**" instructing the interpreter to wait for the arrival of all input files before submitting the job

Appendix Figure 24 Set an input port to be a Collector port


[Job Executable]
[Job I/O]
[JDL
History]
INPUT1
Expects a text
Brow...

View must be selected to make the Parametric details reachable

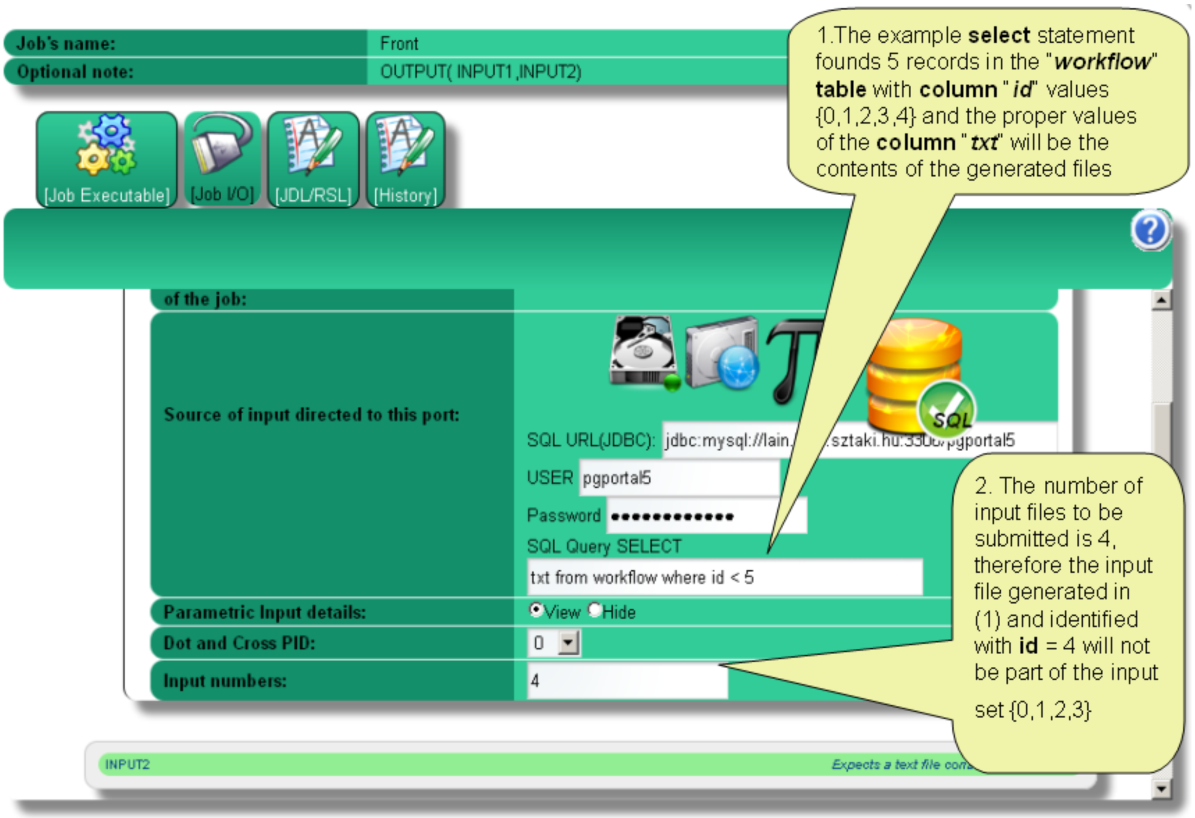
By common **PID** values are the associated jobs joined to a **Cross product** group. By default all ports receive different PID values i.e. input ports have an original **Dot product** relation

Number of files to be elaborated on a genuine input port is determined by "**Input numbers**". The files can be either ***uploaded*** by a special file having the distinguished name "**paramInputs.zip**" or must be enumerated in a **remote grid file catalogue**

Job's name: Front
Optional note: OUTPUT(INPUT1,INPUT2)

Input Port's Internal File Name: INPUT1
Port dependent condition allow… the run of the job: ○View ●Hide
Source of input directed to this port: Rec…ly defined External File N… paramInputs.zip (Stand…d name paramInputs.zip …be regard as PS container) F:\A\paramInputs.zip
Parametric Input details: ●View ○Hide
Dot and Cross PID: 0
Input numbers: 10

Appendix Figure 25 Set an input Port to be PS input Port



Job's name: Front

Optional note: OUTPUT(INPUT1,INPUT2)

of the job:

Source of input directed to this port:

SQL URL(JDBC): jdbc:mysql://lain. .sztaki.hu:3306/pgportal5

USER pgportal5

Password ●●●●●●●●●●●●●

SQL Query SELECT

txt from workflow where id < 5

Parametric Input details: ● View ○ Hide

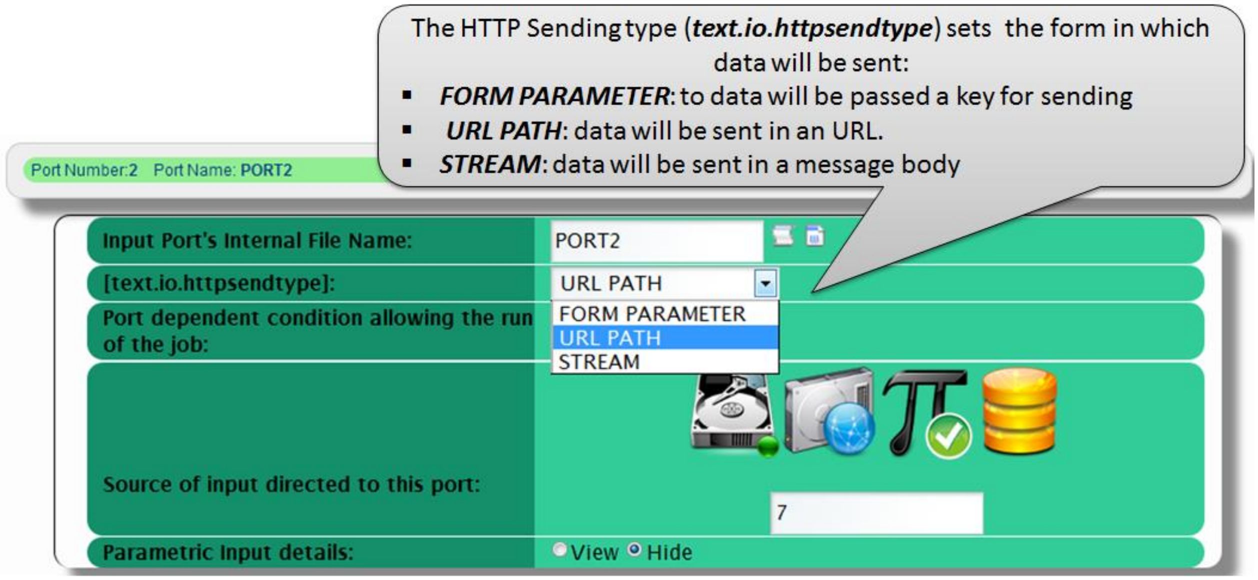
Dot and Cross PID: 0

Input numbers: 4

1.The example **select** statement founds 5 records in the "***workflow***" **table** with **column** "*id*" values {0,1,2,3,4} and the proper values of the **column** "*txt*" will be the contents of the generated files

2. The number of input files to be submitted is 4, therefore the input file generated in (1) and identified with **id** = 4 will not be part of the input set {0,1,2,3}

Appendix Figure 26 Associate an SQL Database to an input Port



The HTTP Sending type (***text.io.httpsendtype***) sets the form in which data will be sent:

- ***FORM PARAMETER***: to data will be passed a key for sending
- ***URL PATH***: data will be sent in an URL.
- ***STREAM***: data will be sent in a message body

Port Number:2 Port Name: **PORT2**

Input Port's Internal File Name: PORT2

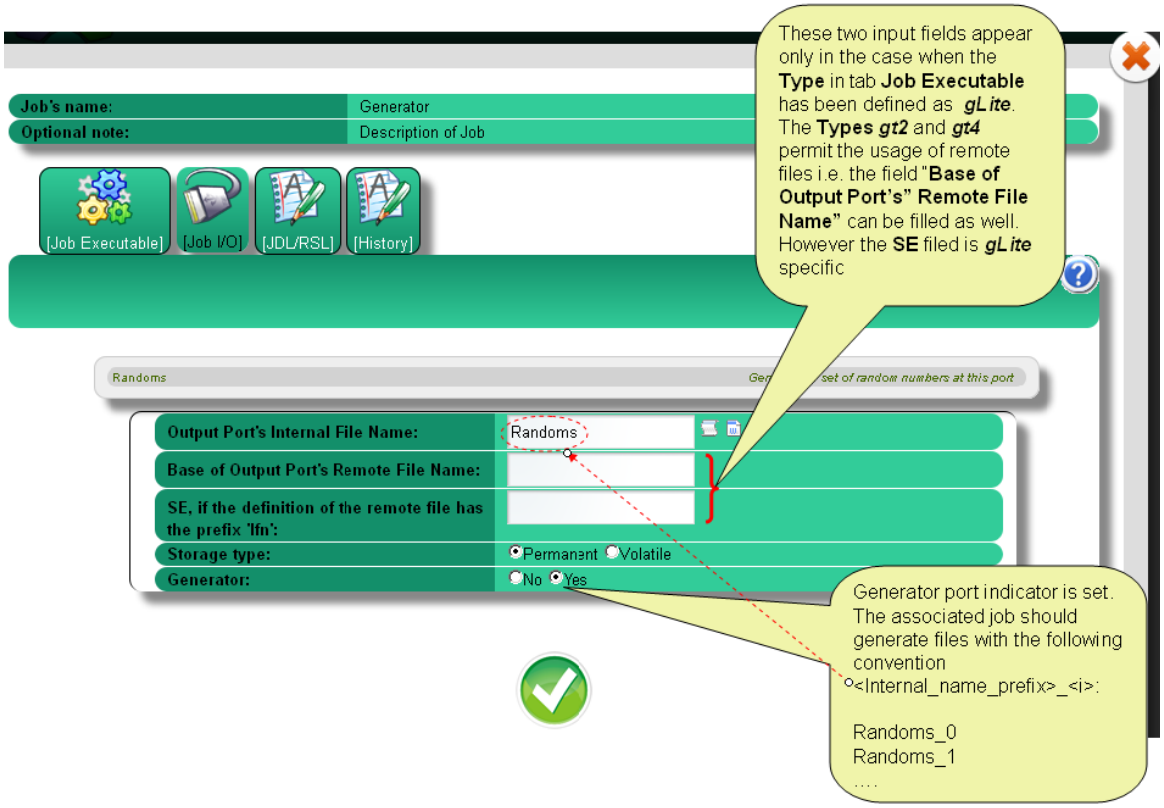
[text.io.httpsendtype]: URL PATH

Port dependent condition allowing the run of the job:

Source of input directed to this port: 7

Parametric Input details: ○ View ● Hide

Appendix Figure 27 Setting input port in case of REST service as resource type


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]

Job's name: Generator
Optional note: Description of Job

Randoms … Ge… set of random numbers at this port

Output Port's Internal File Name: Randoms
Base of Output Port's Remote File Name:
SE, if the definition of the remote file has the prefix 'lfn':
Storage type: ● Permanent ○ Volatile
Generator: ○ No ● Yes

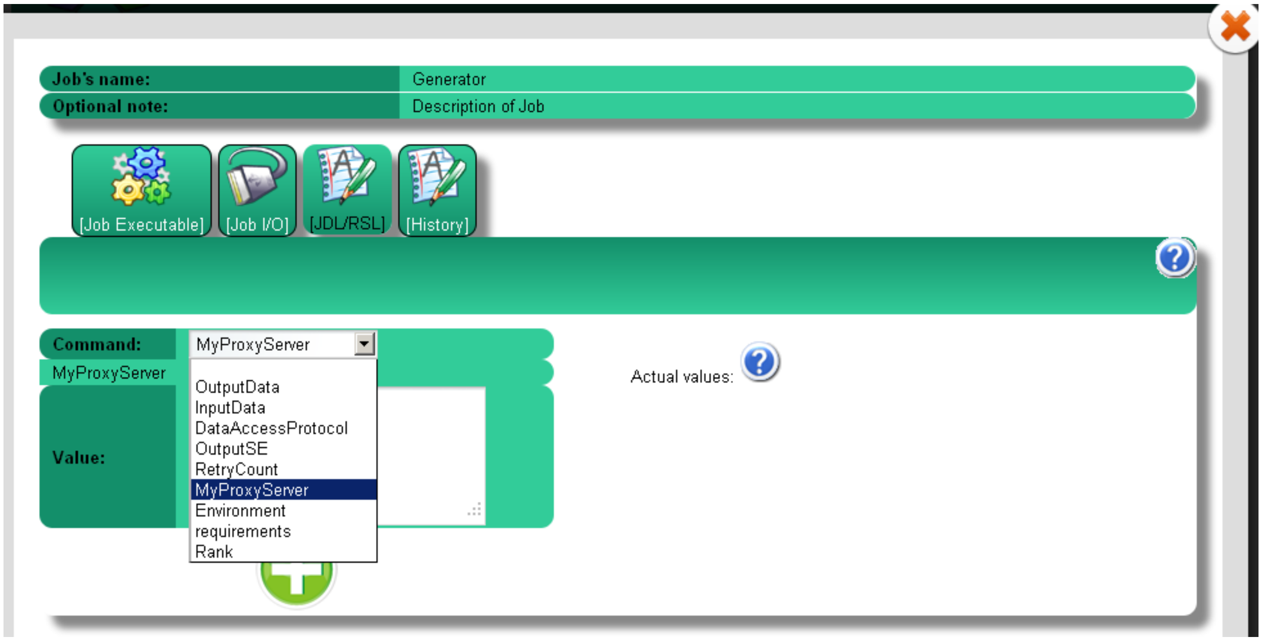
These two input fields appear only in the case when the **Type** in tab **Job Executable** has been defined as ***gLite***. The **Types *gt2*** and ***gt4*** permit the usage of remote files i.e. the field "**Base of Output Port's" Remote File Name"** can be filled as well. However the **SE** filed is ***gLite*** specific

Generator port indicator is set. The associated job should generate files with the following convention <Internal_name_prefix>_<i>:

Randoms_0
Randoms_1
….

Appendix Figure 28 Concrete Configure, Setting Output Ports

3.2.3 The Concrete/Configure/JDL-RSL Tab


[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
OutputData
InputData
DataAccessProtocol
OutputSE
RetryCount
MyProxyServer
Environment
requirements
Rank

Job's name: Generator
Optional note: Description of Job

Command: MyProxyServer
MyProxyServer
Value:
Actual values:

Appendix Figure 29 Concrete Configure, JDL/RSL editor

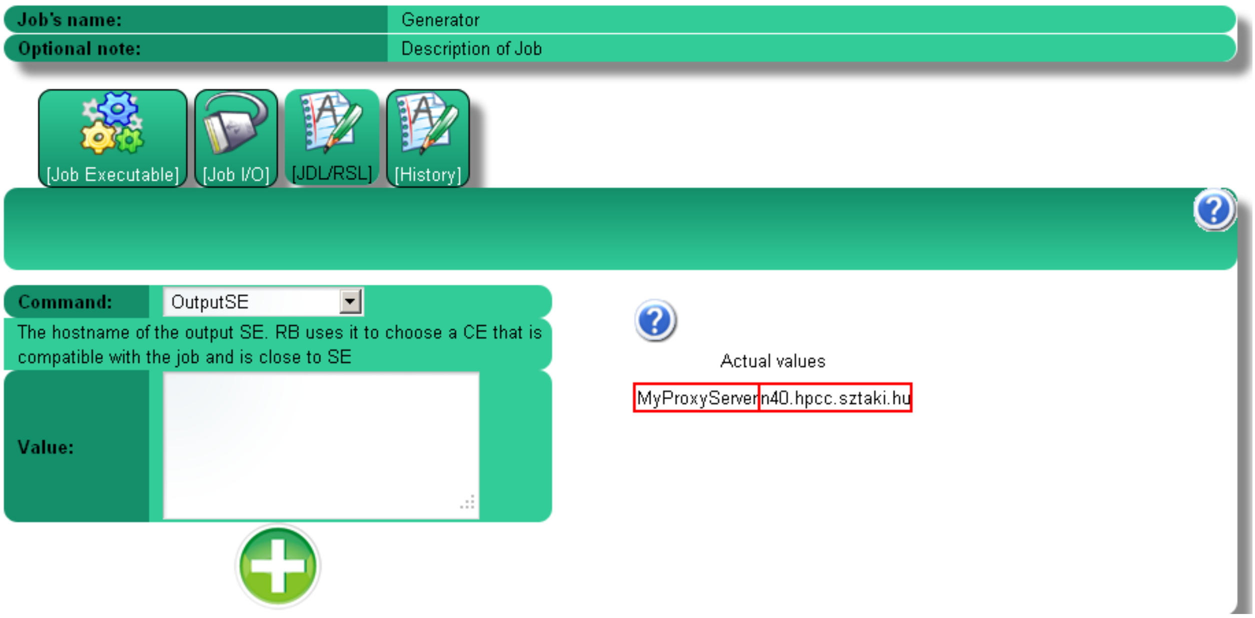
In this form grid and middleware specific additional information can be defined.

Traditionally, this information is stored inside of a user edited file meeting the specifications of the proper job descriptor language like JDL, RSL, etc. The gUSE generates these Job descriptors automatically extended by the entries the user has defined with the assistance of this form explicitly.

These entries are consisting of key-value pairs, where the set of selectable keys is grid/middleware specific (defined by the radio button Type of the sibling form Job Executable) and the value part of the definition is a free string. However these free strings must correspond to the specifications of the respecting job description languages, i.e. the syntax check will be postponed in job submission time. Experienced users may notice that it is the portal Administrator who can define new keys to a given middleware in a XML configuration file. To add an entry the user selects the key from the check list Command, defines the proper value in the input text field and confirms the definition by clicking on the button Add.

The deletion is executed the same way: the entry is added repeatedly but this time with an empty string as value. Please remember that closing of the JDL/RSL settings of the job does not ensure the saving/updating of the workflow in itself: The user must hit the *Save on Server* button in the "parent window" before leaving the workflow configuration.

3.2.3.1 The Concrete/Configure/JDL-RSL/Actual values Function



Job's name: Generator

Optional note: Description of Job

Command: OutputSE

The hostname of the output SE. RB uses it to choose a CE that is compatible with the job and is close to SE

Value:

Actual values

MyProxyServer	n40.hpcc.sztaki.hu

Appendix Figure 30 Concrete Configure, JDL/RSL editor with existing settings

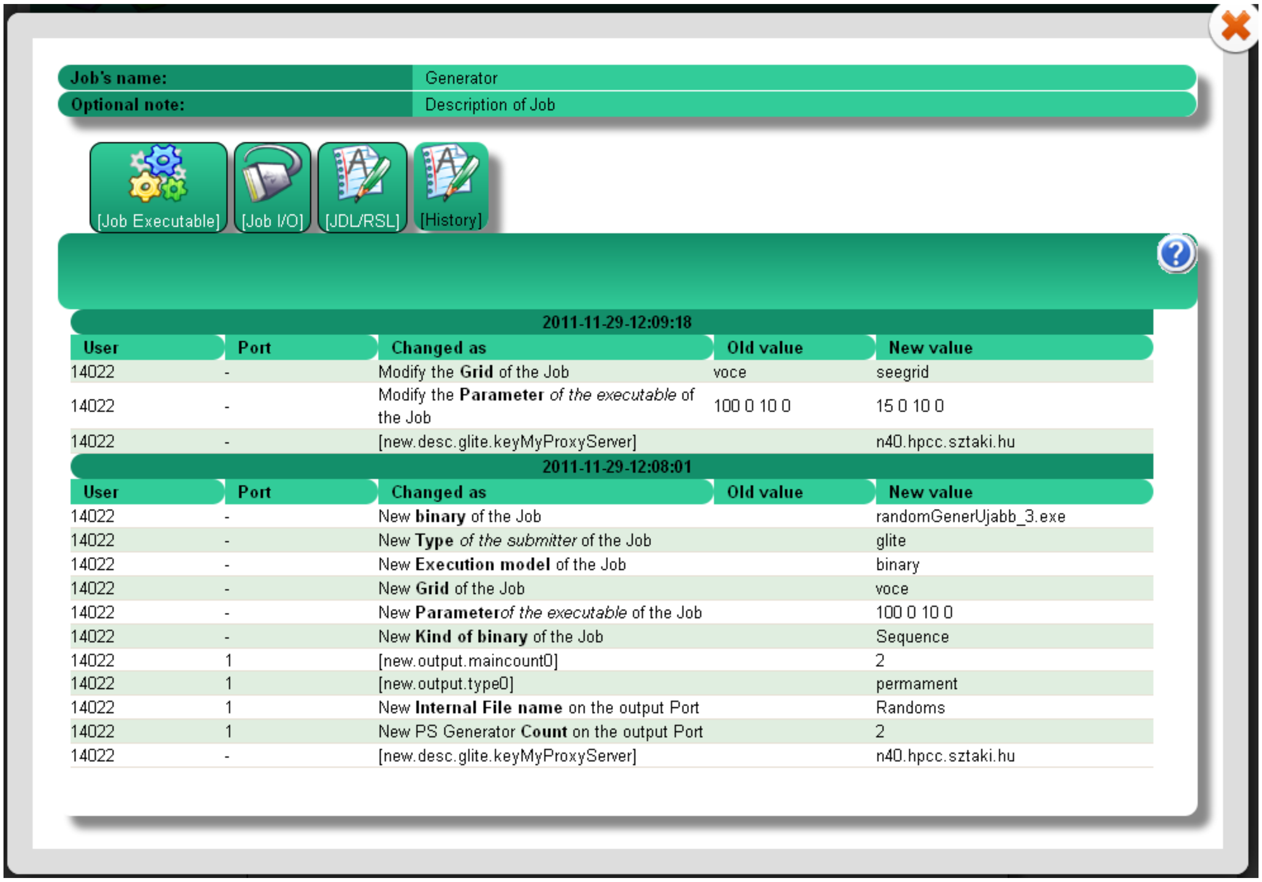
Actual values of the JDL /RSL table with their proper keys are listed in the red framed table.

To redefine or delete an existing element:

1. select the proper key from the *Command* checklist
2. define the new – in the case of deletion empty – value in the *Value* input text field
3. hit the *Add* button

Please, remember that *Closing of the JDL/RSL* settings of the job does not ensure the saving/updating of the workflow in itself: the user must hit the *Save on Server* button in the "parent window" before leaving the workflow configuration

3.2.4 The Concrete/Configure/Job Configuration History Tab



Job's name:	Generator
Optional note:	Description of Job

2011-11-29-12:09:18

User	Port	Changed as	Old value	New value
14022	-	Modify the **Grid** of the Job	voce	seegrid
14022	-	Modify the **Parameter** *of the executable* of the Job	100 0 10 0	15 0 10 0
14022	-	[new.desc.glite.keyMyProxyServer]		n40.hpcc.sztaki.hu

2011-11-29-12:08:01

User	Port	Changed as	Old value	New value
14022	-	New **binary** of the Job		randomGenerUjabb_3.exe
14022	-	New **Type** *of the submitter* of the Job		glite
14022	-	New **Execution model** of the Job		binary
14022	-	New **Grid** of the Job		voce
14022	-	New **Parameter***of the executable* of the Job		100 0 10 0
14022	-	New **Kind of binary** of the Job		Sequence
14022	1	[new.output.maincount0]		2
14022	1	[new.output.type0]		permament
14022	1	New **Internal File name** on the output Port		Randoms
14022	1	New PS Generator **Count** on the output Port		2
14022	-	[new.desc.glite.keyMyProxyServer]		n40.hpcc.sztaki.hu

Appendix Figure 31 Concrete Configure, Job Configuration History

Job history is a logbook where the time stamped changes of the configuration of the given job are recorded and displayed.

- The logbook is backed by an SQL database.
- The logbook is a sequence of items which are listed in time descending order.

An item is headed by the time stamp and lists the changed members. The time stamp remembers the event of user command execution to save the workflow containing the given job on the server (via *Save on Server* button)

Only the changed configuration parameters will be listed identified by the following fields:

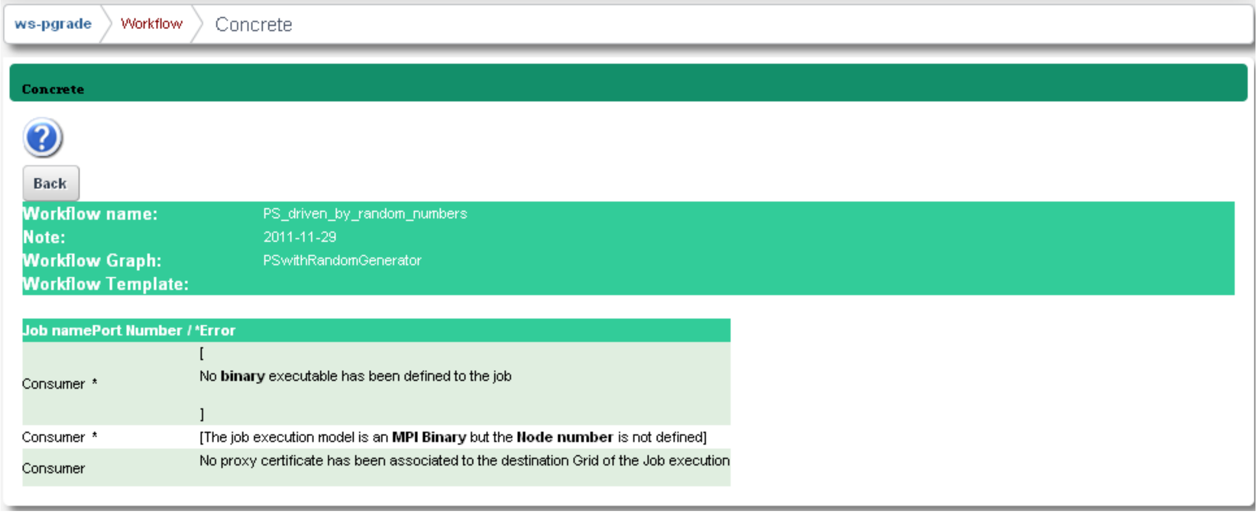
- user: internal identifier of the user. This field will be common for each parameter of the given entry

- port: port number - when applicable i.e. the parameter belongs to a given port
- key: internal identifier of the job level or port level based parameter
- old value: old value of the parameter (if any)
- new value: changed value of the parameter in the stamped time.

The usage of the logbook is restricted by the fact, that the prehistory of the uploaded or imported workflows is not preserved for the time being.

Consequently, the name appearing in the field "*user*" – for the time being – must be identical with the name of the user just being logged in.

3.3 The Concrete/Info Function



Workflow name: PS_driven_by_random_numbers
Note: 2011-11-29
Workflow Graph: PSwithRandomGenerator
Workflow Template:

Job name	Port Number / *	Error
Consumer	*	[No **binary** executable has been defined to the job]
Consumer	*	[The job execution model is an **MPI Binary** but the **Node number** is not defined]
Consumer		No proxy certificate has been associated to the destination Grid of the Job execution

Figure 32 Concrete Menu – Info

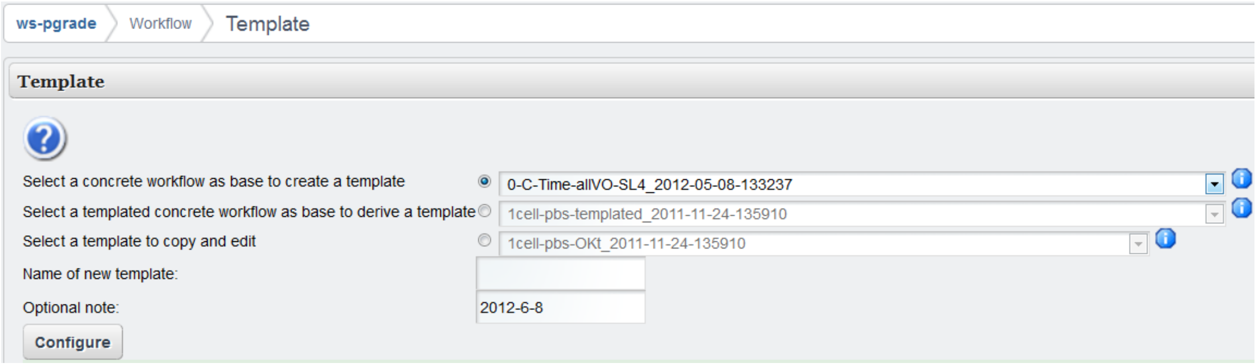
The page Info opened by the button Info reveals the eventually found "syntactical" errors of a workflow. These errors fall in two categories:

1. There is no living (not expired) proxy certificate associated to the named job.
2. An obligatory configuration parameter within a job is missing.

There is a separate line for each found error, and the corresponding item has three fields:

1. Job name: locating the place of error within the workflow
2. Port Number / *: Auxiliary information, if necessary. It may be for example the port number to locate a port if the error belongs to a given port, or the name of Grid in case of certificate problem
3. Error: Verbose description of error.

4. The Template Menu



Select a concrete workflow as base to create a template ● 0-C-Time-allVO-SL4_2012-05-08-133237

Select a templated concrete workflow as base to derive a template ○ 1cell-pbs-templated_2011-11-24-135910

Select a template to copy and edit ○ 1cell-pbs-OKt_2011-11-24-135910

Name of new template:

Optional note: 2012-6-8

Appendix Figure 4.1 Template Menu – Create a Template

The term **template** is the main abstraction in the gUSE to support the reusability of the workflows. Shortly speaking a template is a generic workflow where some configuration parameter are fixed forever, so when a template will be used to define a new workflow the user will be helped substantially by inheriting the knowledge frozen in the (hopefully tested) template and being not able to spoil the safe settings.

The lifecycle of a template spans two main phases:

1. Creating a new named template from a workflow regarded to be "good". (This activity is done on this *Workflow/Template* tab)
2. Applying the template to create a new workflow (by selecting the "*Template*" of the radio button "*Create a workflow from a*" in the *Workflow/Create Concrete* tab).

It must be noticed that for safety reason only workflows having been created from Templates can be used as embedded workflows. (See that only such Workflow can be selected in a Job configuration i.e. when the Job execution model is "*Interpretation of job as Workflow*").

The *Workflow/Template* tab: The existing Templates are listed and maintained in the tab Workflow/Template, further the creation of a new Template can be initialized here as well.

1. Template creation
   - Starting point is an existing Workflow or Template. Certainly this Workflow might have been created by the help of a different Template (lets name it "Ancestor Template"). In an even more special case we may want to reserve all fixed settings of the "*Ancestor Template*".
     - This operation is called derivation and discriminated by selecting the radio button setting: "*Select a templated concrete workflow as base to derive a template*".
     - In the alternate case the user selects one from the full set of Workflows ("Select a concrete workflow as base to create a template") and in the subsequent configuration process any parameter can be freed or fixed according user convenience independently of the existence of an eventual "Ancestor Template".

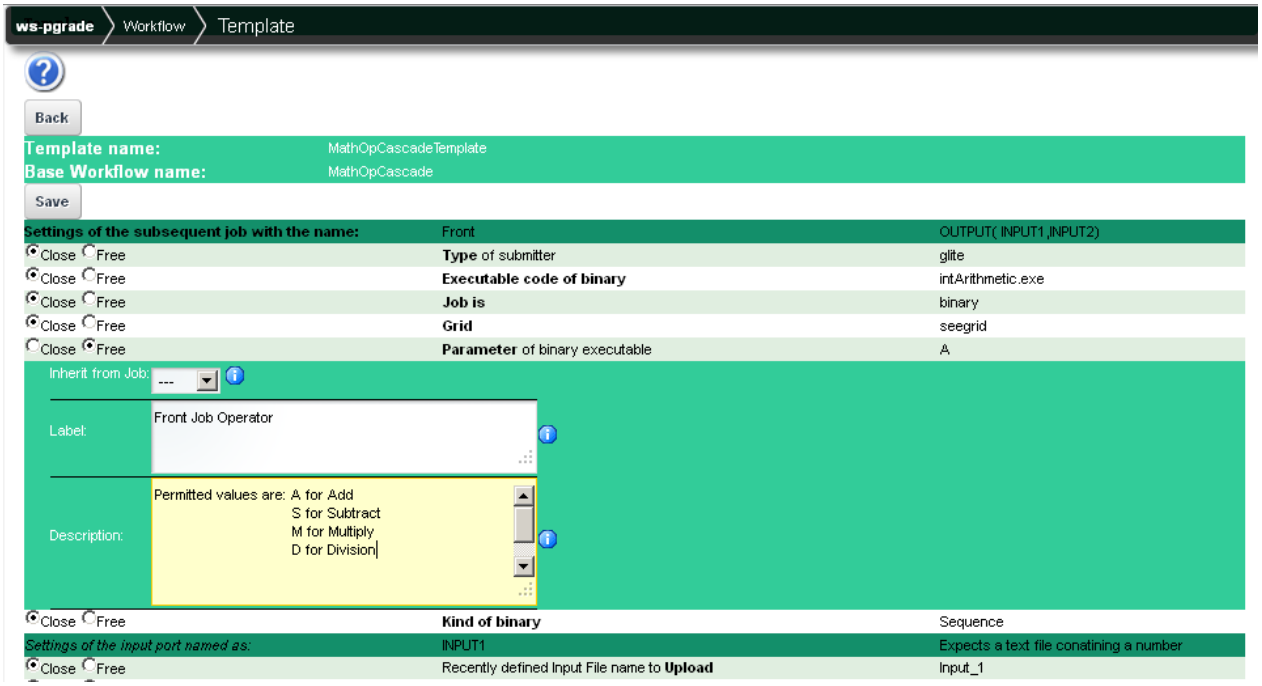
    - In the third case "Select a template to copy and edit" the user selects an existing Template with its default settings. These settings can be modified in the subsequent Configure phase. This feature can be used to edit a given template: A temporary template will be created from the original and saved after the changing the inherited settings; the original template will be deleted and recreated by using the temporary template.
  - The new template to be created must have a distinguished name (For the time being – because of historical causes – workflows and templates have a common name space). This must be defined in the input field of the label Name of new template.
  - The hitting of button Configure opens the form where all individual parameters of the base workflow are listed and about the closure of the yet free ones can be decided upon. Please, note that the configuration must be confirmed by the *Save* button.
2. Template maintenance: Existing templates can be
   - deleted from the portal server (*Delete* button)
   - downloaded (in form of a compressed file) from the portal server to the machine of the client (*Download* button).

Subsequent upload can be done in the *Workflow/Upload* tab - export in the repository common among all users of the portal (*Export* button). (Subsequent import can be done by any anyone accessing the portal using the *Workflow/Import* tab).

Note: There is no *Edit* operation to change the settings of a template. The reason is safety: not to invite the user to change a Template after the time there are existing workflows "stamped" by the properties of the given template.

However, there is a workaround: Let be T1 the Template to be "changed" and W_T1 the Workflow created by this template. Then by the creation of new template T2 we apply W_T1 as base - in the not derivation regime. If we desperately need the renaming of T2 to T1 then we have to delete T1 (certainly with all eventually referenced workflows including W_T1) and repeat the whole process for W_T2 the Workflow which has been created using T2.

4.1 The Template/Configure Function



Template name: MathOpCascadeTemplate
Base Workflow name: MathOpCascade

Settings of the subsequent job with the name:	Front	OUTPUT(INPUT1 ,INPUT2)
● Close ○ Free	**Type** of submitter	glite
● Close ○ Free	**Executable code of binary**	intArithmetic.exe
● Close ○ Free	**Job is**	binary
● Close ○ Free	**Grid**	seegrid
○ Close ● Free	**Parameter** of binary executable	A

Inherit from Job: ---
Label: Front Job Operator
Description: Permitted values are: A for Add
S for Subtract
M for Multiply
D for Division

● Close ○ Free	**Kind of binary**	Sequence
Settings of the input port named as:	INPUT1	Expects a text file conatining a number
● Close ○ Free	Recently defined Input File name to **Upload**	Input_1

Appendix Figure 4.2 Template Menu – Configuring a Template

On this form all configuration elements of the associated Workflow are listed and the user may decide about the closing (freezing) of each individual elements. As default all element are set "to be closed".

Individual elements can be set to be *Free* indicating that the subsequent user configuring the workflows having been generated from the current Template may change the value of the given element. However not each element can be *Free*-ed; elements had been closed in a previous template from which the current template has been "derived" preserve their *Closed* state.

The list contains three features for each element - displayed as columns:

- The locket status - *Close/Free* or *Closed* if the locket status cannot be changed
- The job/port based symbolic identifier of the given element as it appears in the proper configuration.
- The value (or setting) of the given element.

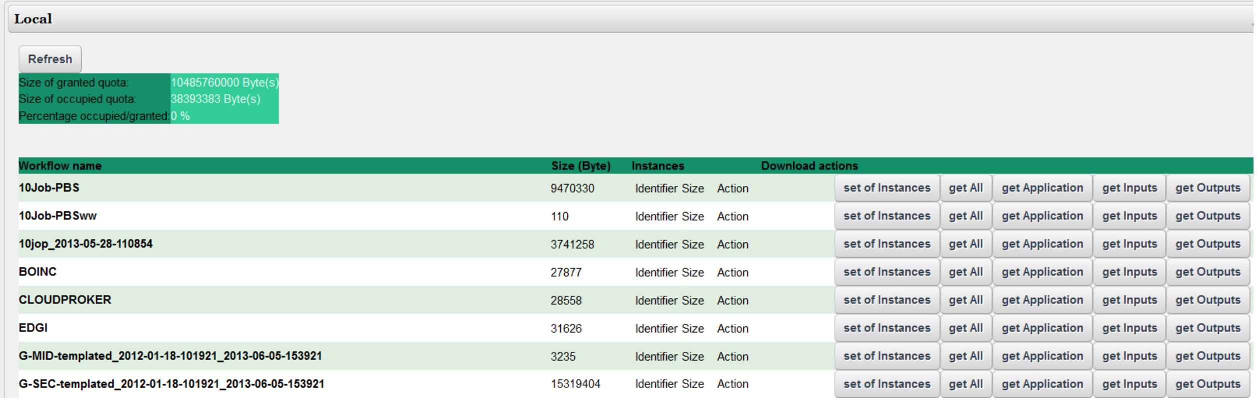
If the user judges an element to be changeable by selecting the *Free* radio button three additional input fields appear, which - in given cases - may be filled:

- Inherit from Job:
- Label:
- Description:

Note*:* *Label* and *Description* can be filled for the notification of a subsequent Non-advanced user: Non-advanced users do not build a workflow the traditional way: They use a template to generate a single simplified Form, where all parameters of the workflow to be build and requested to be defined by the non-advanced user is listed. The application dependent *Name* and *Description* belonging to each requested input value of this form can be prepared by defining *Label* and *Description* respectively.

"Inherit from Job" is a short hand. If the user has defined "Label" and "Description" in a different job for the same field, and wants the texts associated to "Label" and "Description" to be replicated here, then references the given job. Do not forget to confirm the Configuration by *Save* button.

5. The Storage Menu



Size of granted quota:	10485760000 Byte(s)
Size of occupied quota:	38393383 Byte(s)
Percentage occupied/granted:	0 %

Workflow name	Size (Byte)	Instances	Download actions
10Job-PBS	9470330	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
10Job-PBSww	110	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
10jop_2013-05-28-110854	3741258	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
BOINC	27877	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
CLOUDPROKER	28558	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
EDGI	31626	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
G-MID-templated_2012-01-18-101921_2013-06-05-153921	3235	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs
G-SEC-templated_2012-01-18-101921_2013-06-05-153921	15319404	Identifier Size Action	set of Instances get All get Application get Inputs get Outputs

Appendix Figure 5.1 The Storage menu

This page enables the downloading of workflows, workflow instances or parts of them from the portal server into the user's desk top machine.

Note: The selected object will be downloaded in form of a single compressed file.

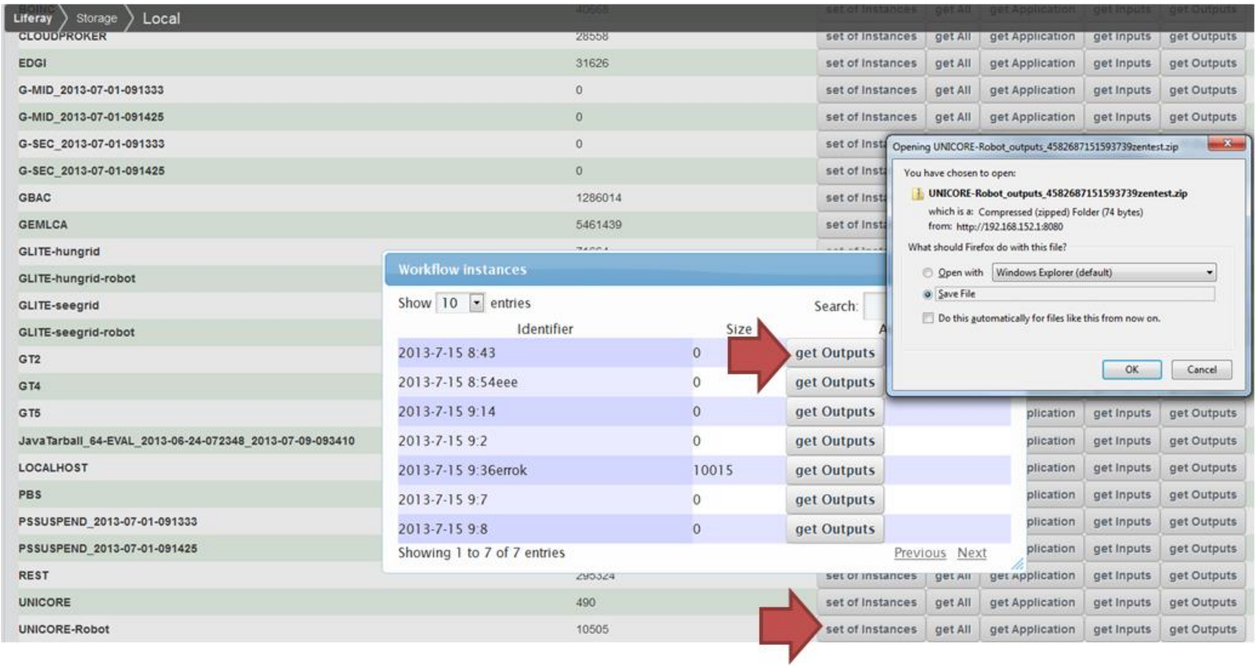
This format enables the current or a different user to upload a selected workflow subsequently from a local archive into the Portal Server using the *Workflow/Upload* tab. The main differences between the *Upload/Download* and the *Export/Import* mechanisms are the following:

- *Upload/Download* happens between the Portal Server and the client machine of the current user, where Export/Import connects the user's storage area on the Portal Server with the Repository which is common and visible among all users.
- Further, with the help of download data, which are different from pure workflow definition (as input files, output files, log files) can be downloaded as well.

The starting point of accessing the downloadable items is the list of existing workflows.

1. **Instances**: As several workflow instances may belong to a single workflow, the user may decide to download only the information which belongs to a single workflow instance. These operations are grouped under the column labeled as *Instances*. Having selected a single instance by button *set of Instances,* an additional operation can be selected:

- by hitting the button *get Outputs* just the local output files having been produced by given workflow run can be reached.



CLOUDPROKER	28558
EDGI	31626
G-MID_2013-07-01-091333	0
G-MID_2013-07-01-091425	0
G-SEC_2013-07-01-091333	0
G-SEC_2013-07-01-091425	0
GBAC	1286014
GEMLCA	5461439
GLITE-hungrid	
GLITE-hungrid-robot	
GLITE-seegrid	
GLITE-seegrid-robot	
GT2	
GT4	
GT5	
JavaTarball_64-EVAL_2013-06-24-072348_2013-07-09-093410	
LOCALHOST	
PBS	
PSSUSPEND_2013-07-01-091333	
PSSUSPEND_2013-07-01-091425	
REST	295324
UNICORE	490
UNICORE-Robot	10505

Workflow instances

Show 10 entries

Identifier	Size	
2013-7-15 8:43	0	get Outputs
2013-7-15 8:54eee	0	get Outputs
2013-7-15 9:14	0	get Outputs
2013-7-15 9:2	0	get Outputs
2013-7-15 9:36errok	10015	get Outputs
2013-7-15 9:7	0	get Outputs
2013-7-15 9:8	0	get Outputs

Showing 1 to 7 of 7 entries

Opening UNICORE-Robot_outputs_4582687151593739zentest.zip

You have chosen to open:

UNICORE-Robot_outputs_4582687151593739zentest.zip

which is a: Compressed (zipped) Folder (74 bytes)

from: http://192.168.152.1:8080

What should Firefox do with this file?

○ Open with Windows Explorer (default)

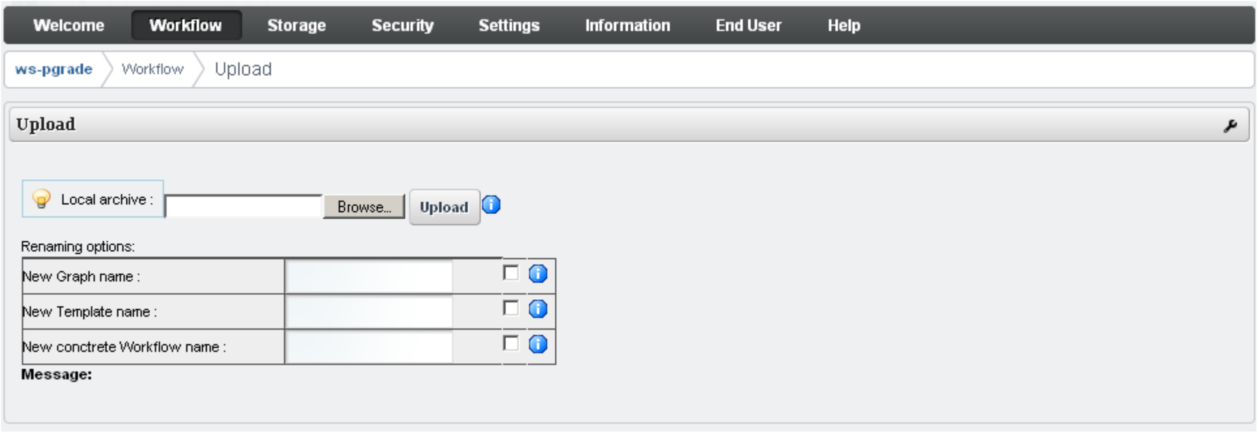
● Save File

☐ Do this automatically for files like this from now on.

Appendix Figure 5.2 The set of Instances function within Storage menu

2. **Workflow**: The other kinds of download options refer to the whole workflow and are collected in the column labeled as *Download actions*. It means that the referenced parts of all eventual workflow instances will be downloaded as well:
   - By hitting the *get All* button - all data belonging to the workflow will be downloaded.
   - By hitting the *get Application* button – only the workflow (together with input files) will be downloaded.
   - By hitting the *get Inputs* button - the local input files of all instances can be downloaded.
   - By hitting the *get Outputs* button - the local output files of all instances can be downloaded.

6. The Upload Menu


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Workflow
Upload
Upload
Local archive :
Browse...
Upload
Renaming options:
New Graph name :
New Template name :
New conctrete Workflow name :
Message:

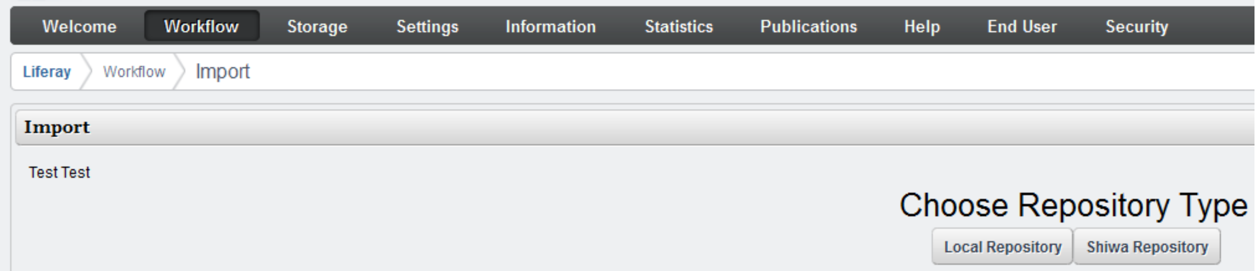
Appendix Figure 6.1 Upload menu

This page enables the uploading of graphs of templates or of workflows from the user's desk top machine into the portal server. In the user's desk top machine an object to be uploaded is stored in a single compressed file, ruled by the syntax determined by a preceding Download operation. The inverse download operations can be found at *Download* button in case of graphs (*Workflow/Graph* tab) and in case of template (*Workflow/Template* tab) and at the *get All* and *get All but logs* buttons in case of workflows (*Workflow/Storage* tab). The uploading of a workflow automatically involves the uploading of the associated Graph and may involve the uploading of a template if the given Workflow has been defined on the basis of a Template. Upon upload the referenced graph, template and workflow objects – if no extra measure is taken - will be stored with their original names among the other objects of their own types in the proper name spaces. Name collisions are not permitted and the new objects with colliding names are refused. To avoid name collisions the user has the option to change the proper (graph, template, and workflow) names of the object to be uploaded.

The name of the compressed file to be uploaded can be defined either by typing its path in the input field *Local Archive* or located by the file browser *Browse*. The operation must be confirmed by hitting the button Upload. The optional renaming of the objects (done in the proper *New Graph name, New Template name, New concrete Workflow name* input fields) must be preceded by setting of the proper check boxes.

7. The Import Menu

The import function of WS-PGRADE (expressed by *Import* menu that you can access from *Workflow/Import* menu) provides solution to import different workflows. This function consists of two main way of importation depending on which repository segment you want to use. You can choose the *Local Repository* if the target workflow shared in local gUSE/WS-PGRADE community. You can choose *SHIWA Repository* if the target workflow shared in SHIWA project community. (About sharing/exporting function see Appendix chapter 11.)

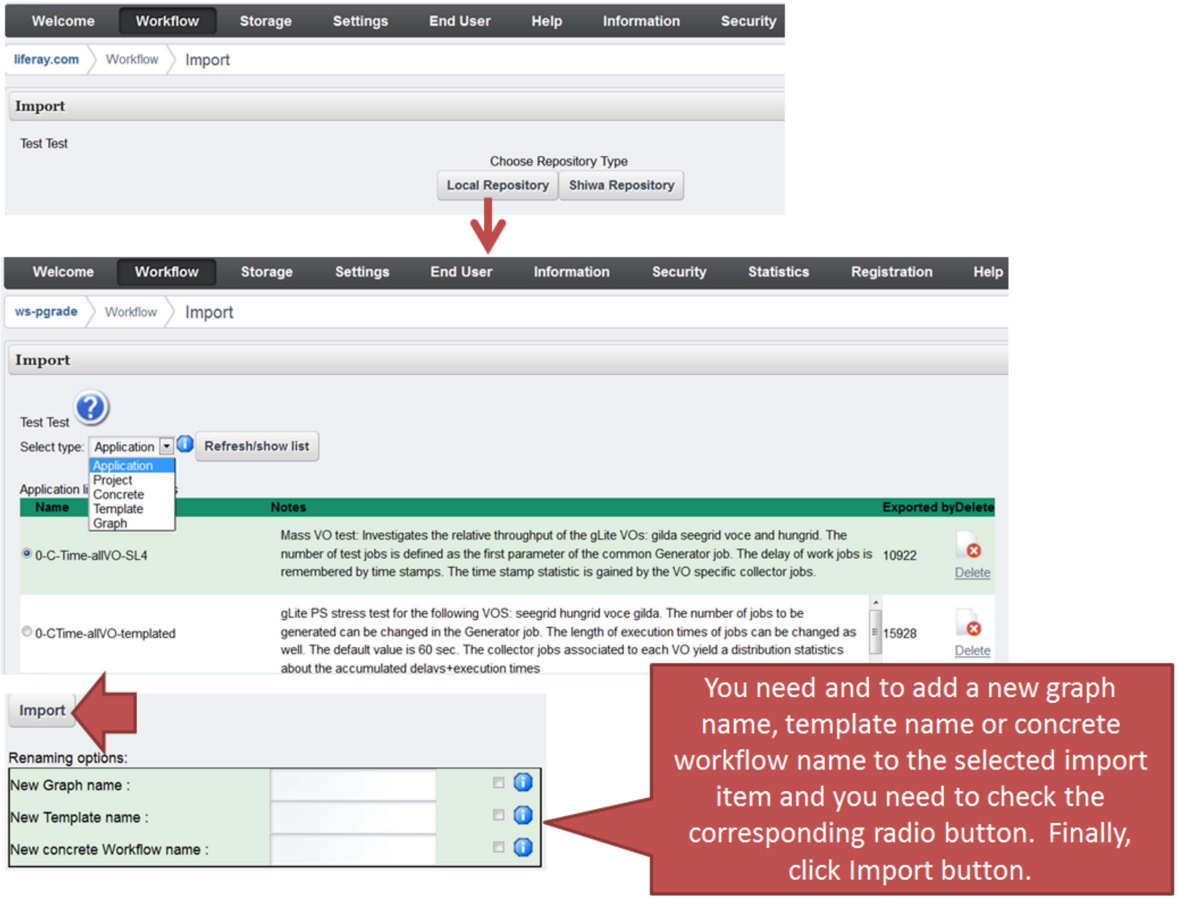


Appendix Figure 7.1 The start-up window within Import menu with two possible options

Import from Local Repository (Appendix Figure 7.2): The appearing page after clicking *Local Repository* button on startup shows (and permits further operations on) the selected segment of the Repository which is common among the users of the gUSE/WS-PGRADE Portal. Five different kinds of objects can be distinguished and selected as a segment:

- **Application** (default value)
- **Project**
- **Concrete workflow**
- **Template**
- **Graph**

The term *Application* means the definition of a full and environment free tested workflow (which involves the definition(s) of eventual embedded workflows i.e. transitive closure of reference sequences of them including Graphs and Templates). The term *Project* means the "under construction" state of an Application i.e. it must not be full and tested however it contains the definition(s) of embedded workflow(s) if it is/they are available. The term *Workflow* involves the definition of its Graph and may involve the definition of a Template if the workflow has been defined on the base of that Template. The objects of the repository has been created by proper export operations (*Export* button) issued in *Workflow/Graph, Workflow/Template* and *Workflow/Concrete* tabs respectively. It must be remembered that all these objects have been created with optional verbose comments which are readable here in the column labeled as *Notes*.


Welcome
Workflow
Storage
Settings
End User
Help
Information
Security
liferay.com
Workflow
Import
Import
Test Test
Choose Repository Type
Local Repository
Shiwa Repository
Welcome
Workflow
Storage
Settings
End User
Information
Security
Statistics
Registration
Help
ws-pgrade
Workflow
Import
Import
Test Test
Select type:
Application
Refresh/show list
Application
Project
Concrete
Template
Graph
Application li
Import
Renaming options:

Name	Notes	Exported by	Delete
● 0-C-Time-allVO-SL4	Mass VO test: Investigates the relative throughput of the gLite VOs: gilda seegrid voce and hungrid. The number of test jobs is defined as the first parameter of the common Generator job. The delay of work jobs is remembered by time stamps. The time stamp statistic is gained by the VO specific collector jobs.	10922	Delete
○ 0-CTime-allVO-templated	gLite PS stress test for the following VOS: seegrid hungrid voce gilda. The number of jobs to be generated can be changed in the Generator job. The length of execution times of jobs can be changed as well. The default value is 60 sec. The collector jobs associated to each VO yield a distribution statistics about the accumulated delavs+execution times	15928	Delete

New Graph name :		☐
New Template name :		☐
New concrete Workflow name :		☐

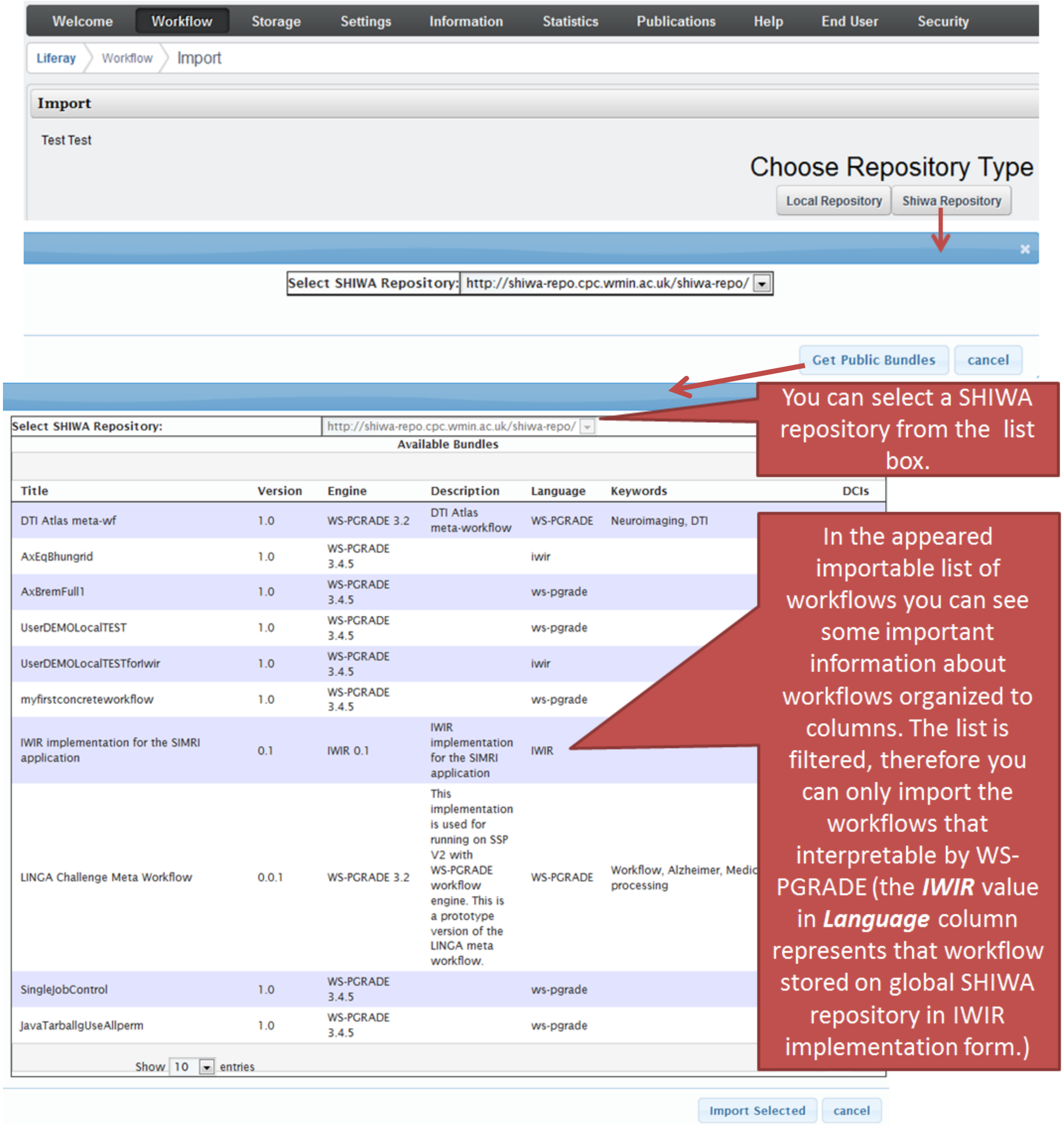
You need and to add a new graph name, template name or concrete workflow name to the selected import item and you need to check the corresponding radio button. Finally, click Import button.

Appendix Figure 7.2 Import function 1: import from local repository

The next important point to mention is that the export command of *Workflow/Concrete* (see Appendix chapter 11) is branching to export the workflow as a common workflow or as an *Application* or as a *Project*. The base operation on this page is the Import of the selected object. However the distinguished administrator user "root" and "owner" of the given item has the right to *Delete* a repository item as well. The "owner" of the given object is the user who has exported it.

Importing means the copy of the selected object from the repository into the proper allocated user's storage area on the Portal Server. Upon import the referenced graph, template and workflow objects – if no extra measure is taken - will be stored with their original names among the other objects of their own types in the proper name spaces.

Warning: Name collisions are not permitted and the new objects with colliding names are refused. To avoid name collisions the user has the option to change the proper (Graph, Template, and Workflow) names of the object to be imported. It is important to note that the eventual embedded objects cause no name collision as their names will be automatically extended upon import in order to make them unique in the given name spaces.


Welcome
Workflow
Storage
Settings
Information
Statistics
Publications
Help
End User
Security
Liferay
Workflow
Import
Import
Test Test
Choose Repository Type
Local Repository
Shiwa Repository
Select SHIWA Repository: http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/
Get Public Bundles
cancel
Show 10 entries
Import Selected
cancel

Select SHIWA Repository: http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/

Available Bundles

Title	Version	Engine	Description	Language	Keywords	DCIs
DTI Atlas meta-wf	1.0	WS-PGRADE 3.2	DTI Atlas meta-workflow	WS-PGRADE	Neuroimaging, DTI	
AxEqBhungrid	1.0	WS-PGRADE 3.4.5		iwir		
AxBremFull1	1.0	WS-PGRADE 3.4.5		ws-pgrade		
UserDEMOLocalTEST	1.0	WS-PGRADE 3.4.5		ws-pgrade		
UserDEMOLocalTESTforIwir	1.0	WS-PGRADE 3.4.5		iwir		
myfirstconcreteworkflow	1.0	WS-PGRADE 3.4.5		ws-pgrade		
IWIR implementation for the SIMRI application	0.1	IWIR 0.1	IWIR implementation for the SIMRI application	IWIR		
LINGA Challenge Meta Workflow	0.0.1	WS-PGRADE 3.2	This implementation is used for running on SSP V2 with WS-PGRADE workflow engine. This is a prototype version of the LINGA meta workflow.	WS-PGRADE	Workflow, Alzheimer, Medic processing	
SingleJobControl	1.0	WS-PGRADE 3.4.5		ws-pgrade		
JavaTarballgUseAllperm	1.0	WS-PGRADE 3.4.5		ws-pgrade		

You can select a SHIWA repository from the list box.

In the appeared importable list of workflows you can see some important information about workflows organized to columns. The list is filtered, therefore you can only import the workflows that interpretable by WS-PGRADE (the ***IWIR*** value in ***Language*** column represents that workflow stored on global SHIWA repository in IWIR implementation form.)

Appendix Figure 7.3 Import function 2: import from SHIWA Repository

The user activity includes 3 subsequent steps:

1. Select the required *Repository* segment by the check list Select type: and confirmed by the button *Refresh*/show list.
2. Select the object to be manipulated the left side radio button. This step may include the optional prescription of renaming of the imported objects (done in the proper *New Graph name, New Template name, New concrete Workflow name* input fields) which must be preceded by setting of the proper check boxes.

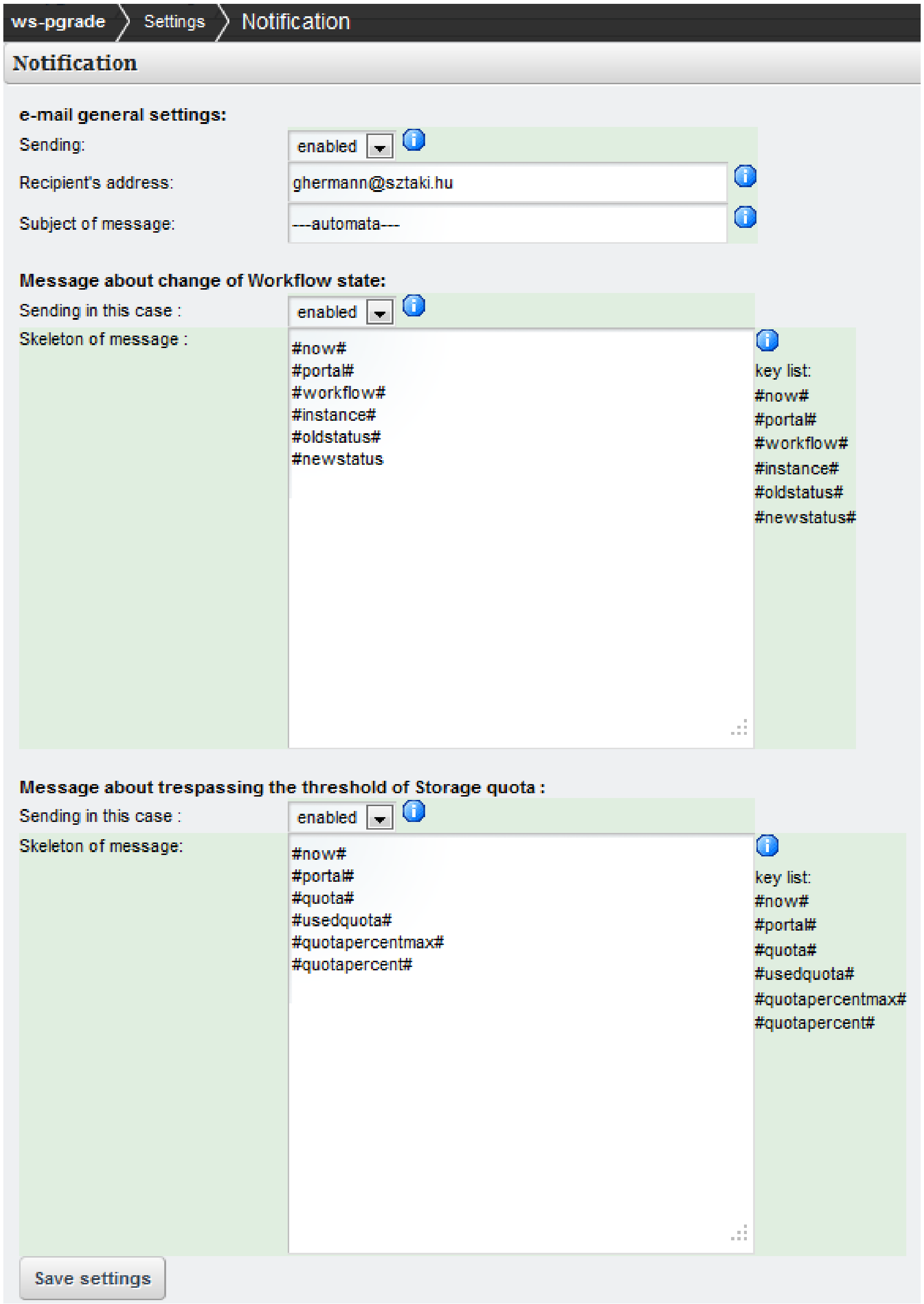
3. Selection the command to be executed by the *Select action type* check list and confirmed by *Execute* button.

Import from SHIWA repository (Appendix Figure 7.3): In this case workflows will be accessible on WS-PGRADE-based language or on **SHIWA IWIR** language. (It depends on in which implementation formats have been shared workflows earlier.)

In order to import workflows you can choose the **SHIWA Repository** option at startup window, then you can select a SHIWA repository and get public bundles (bundle means workflows together with input files, dependencies and descriptions) as shown on Appendix figure 7.3. The import process will be enforced by the clicking on *Import Selected* button.

The automatic conversion of workflow for WS-PGRADE environment is immediately created after importation process and therefore you can check the correctness of importation directly on the imported workflow through *Workflow/Concrete* menu.

8. The Notification Menu



Notification

e-mail general settings:

Sending: enabled

Recipient's address: ghermann@sztaki.hu

Subject of message: ---automata---

Message about change of Workflow state:

Sending in this case : enabled

Skeleton of message :

```
#now#
#portal#
#workflow#
#instance#
#oldstatus#
#newstatus
```

key list:
#now#
#portal#
#workflow#
#instance#
#oldstatus#
#newstatus#

Message about trespassing the threshold of Storage quota :

Sending in this case : enabled

Skeleton of message:

```
#now#
#portal#
#quota#
#usedquota#
#quotapercentmax#
#quotapercent#
```

key list:
#now#
#portal#
#quota#
#usedquota#
#quotapercentmax#
#quotapercent#

Figure 8.1 The Notification menu

The user may instruct the system to send notification(s) about given state changes, having been caused indirectly or directly by the submission of a workflow:

1. The trespass of a threshold value relating the Storage quota of the user in the gUSE Server is referred as indirect change.

2. Two kinds of direct changes from the point of view are distinguished:
    - The workflow instance reaches an end state ("finished" or "error") from where it may not be moved without manual user action.
    - The global state of the workflow instance has changed (for example from "submitted" to "running", or from "running" to "finished" or to "error").

The notification prescription will not be forwarded to the submissions of the eventual embedded workflows. At present the only way of the notification is a sent e-mail message.

The *Workflow/Notify* tab configuring these messages is structured the following way:

1. E-mail general settings groups the base information needed to send an electronic mail involving the recipient's address, the subject of the message and the overall permission to send any letter. The interested reader may notice that the URL of the SMPT server needed to send the letter can be changed by the Administrator of the gUSE Portal via the proper entry of the file *Services.properties*.
2. Message about change of workflow state is the editable skeleton of the letter sent in the case of an event of direct change category (see above). The user has a further filter possibility to disable/enable these letters by the selecting the proper value of the checklist Sending in this case As a summary the sending of a letter has five conditions controlled by the user:
    1. The proper e-mail address is set
    2. Sending is enabled
    3. Sending in this case is enabled
    4. Upon submitting the workflow on the question "Send e-mail in case" the answer is not "never"
    5. The event listened for has occurred

    The content of the message is free editable in the text area Skeleton of the message.

    The substituting values of the eventual keys inserted in the text will be evaluated in the time of sending the letter.

    These keys and their meanings are the following:

    - **#now#** - Time stamp of event
    - **#portal#** - URL of the portal
    - **#workflow#** - Name of workflow
    - **#instance#** - Identifier of workflow instance
    - **#oldsatus#** - State prior the event
    - **#newsatus#** - State caused by the event
3. Message about trespassing the threshold of storage quota is the editable skeleton of the letter sent in the case of an event of indirect change category (see above). The interested reader may notice that a integer threshold value meaning a ratio of the storage capacity allotted to the user by the administrator of the gUSE portal is set in a proper entry of the file

PGradePortal.properties. It must be noted the system realizes the trespass with a – sometimes long – delay, as it investigates the user quotas periodically and not at any storage requirement.

Note: The system does not suspend any running workflow on quota trespassing exception. However it prohibits manual submitting or editing operations until the quota problem is solved. The user has a further filter possibility to disable /enable these letters by the selecting the proper value of the checklist *Sending* in this case.

As a summary the sending of a letter of this kind has four conditions controlled partly the user:

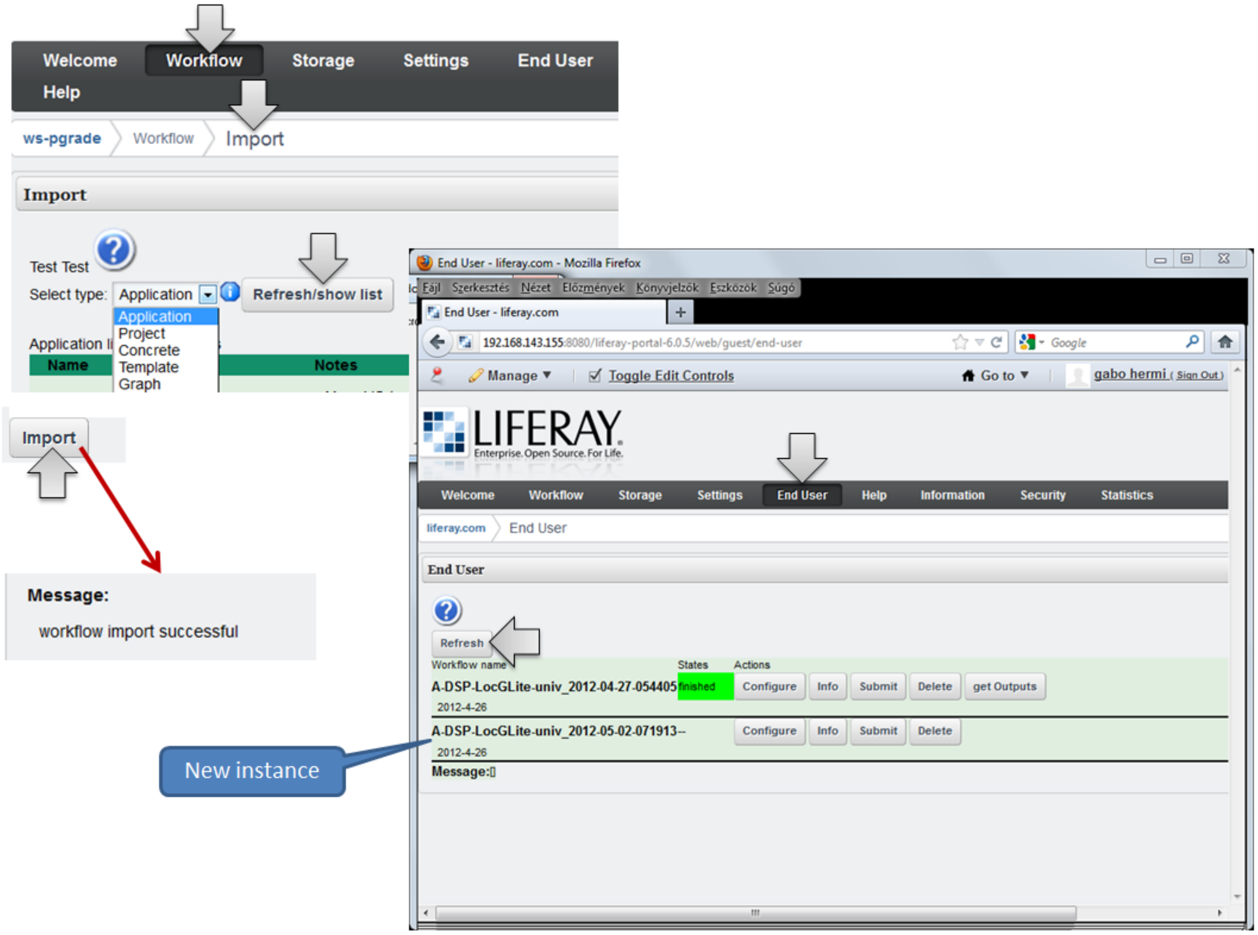
1. The proper e-mail address is set
2. Sending is enabled
3. Sending in this case is enabled
4. The quota checker has found threshold trespass.

The content of the message is free editable in the text area Skeleton of the message. The substituting values of the eventual keys inserted in the text will be evaluated in the time of sending the letter. These keys and their meanings are the following:

- **#now#** - Time stamp of event
- **#portal#** - URL of the portal
- **#quota#** - Storage allotted by the Administrator to the user in the tab Workflow/settings
- **#usedquota#** - Actual storage occupied by the user
- #**quotapercentmax#** - The common threshold value expressed in percent
- #**quotapercent#** - The ratio of "usedquota" and "quota" expressed in percent

4. The settings must be saved hitting the *Save* button settings.

9. The End User Menu


Welcome
Workflow
Storage
Settings
End User
Help
ws-pgrade
Workflow
Import
Import
Test Test
Select type:
Application
Refresh/show list
Application
Project
Concrete
Template
Graph
Name
Notes
Import
New instance
End User - liferay.com - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
End User - liferay.com
192.168.143.155:8080/liferay-portal-6.0.5/web/guest/end-user
Google
Manage
Toggle Edit Controls
Go to
gabo hermi (Sign Out)
LIFERAY
Enterprise. Open Source. For Life.
Welcome
Workflow
Storage
Settings
End User
Help
Information
Security
Statistics
liferay.com
End User
End User
Refresh
Workflow name
States
Actions
Configure
Info
Submit
Delete
get Outputs

Message:

workflow import successful

A-DSP-LocGLite-univ_2012-04-27-054405 finished
2012-4-26

A-DSP-LocGLite-univ_2012-05-02-071913--
2012-4-26

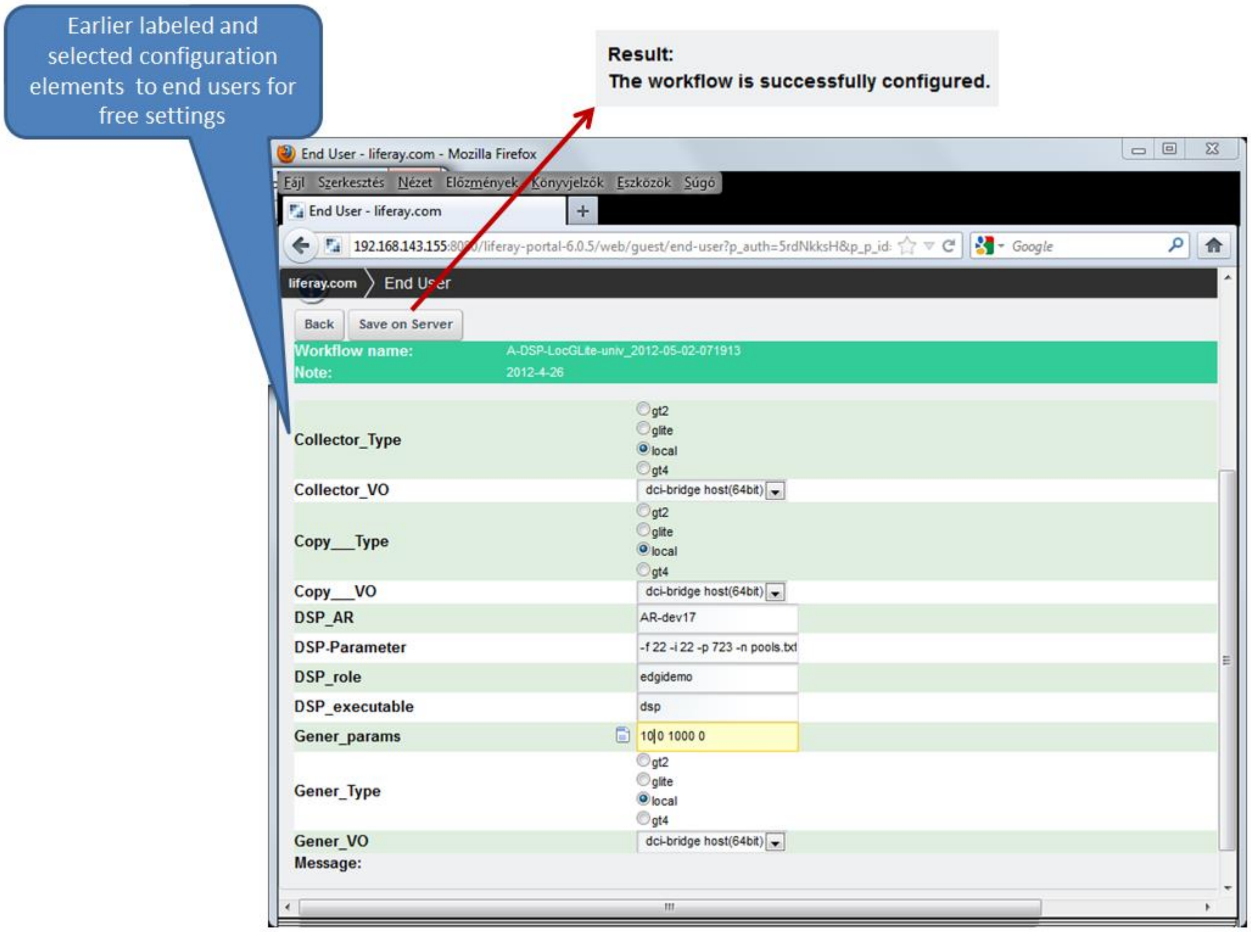
Message:

Appendix Figure 9.1 Workflow import to end users for workflow configuration

This page supports emphatically the inexperienced users - so called end-users - of the WS-PGRADE Portal to configure and submit workflows which have been developed and tested by experts.

The distinction between end-users and common users is done by the administrator of the portal upon Portal User Account requests by permitting different activities selectable from different tab sets available for these two groups of users:

1. The main tab *End User Application* groups the tabs selectable by the end-user.
2. The main tab *Workflow* groups all workflow related manipulation tabs without restriction


End User - liferay.com - Mozilla Firefox
Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
End User - liferay.com
192.168.143.155:8080/liferay-portal-6.0.5/web/guest/end-user?p_auth=5rdNkksH&p_p_id:
Google
liferay.com
End User
Back
Save on Server

Earlier labeled and selected configuration elements to end users for free settings

Result:
The workflow is successfully configured.

Workflow name:	A-DSP-LocGLite-univ_2012-05-02-071913
Note:	2012-4-26
Collector_Type	○ gt2 ○ glite ● local ○ gt4
Collector_VO	dci-bridge host(64bit)
Copy___Type	○ gt2 ○ glite ● local ○ gt4
Copy___VO	dci-bridge host(64bit)
DSP_AR	AR-dev17
DSP-Parameter	-f 22 -i 22 -p 723 -n pools.txt
DSP_role	edgidemo
DSP_executable	dsp
Gener_params	100 1000 0
Gener_Type	○ gt2 ○ glite ● local ○ gt4
Gener_VO	dci-bridge host(64bit)
Message:	

Appendix Figure 9.2 Workflow configuration of end users: filling a template

The tested workflows (Applications) are stored in the common Repository (pushed there by issuing the command export in the *Workflow/Concrete* tab) from where the user can copy them in the own name space by using the tab Import.

Import is accessible either for the experienced users from the developer tab Workflow or for the inexperienced end users from the tab End User Application.

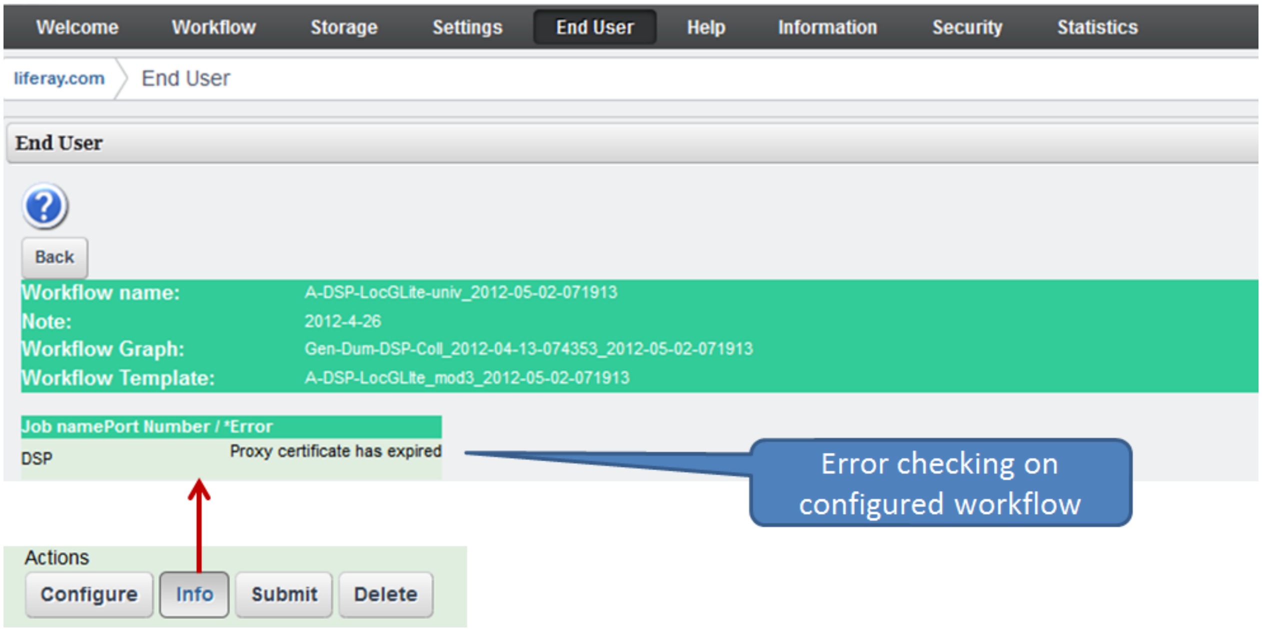
Note: the repository stores not only applications, but only applications will appear in the list shown in this page.

To avoid name collisions, the names of imported objects will be extended by a unique number. A user can perform five kinds of activities associated by proper buttons to a selected application:

1. Configure it by permitted input parameters
2. Check the correctness of the application by Info
3. Submit the Application to execute it on a (remote) resource.
4. Fetch the result of the terminated application by *get Outputs*
5. Deleting the Application.

Beyond that auxiliary activity may be done on different Tabs:

- to fetch a proxy Certificate by Certificates, or
- to archive the executed application with all inputs and settings by Storage


Welcome
Workflow
Storage
Settings
End User
Help
Information
Security
Statistics
liferay.com
End User
End User
Back
Actions
Configure
Info
Submit
Delete
Error checking on configured workflow

Workflow name: A-DSP-LocGLite-univ_2012-05-02-071913
Note: 2012-4-26
Workflow Graph: Gen-Dum-DSP-Coll_2012-04-13-074353_2012-05-02-071913
Workflow Template: A-DSP-LocGLite_mod3_2012-05-02-071913

Job namePort Number / *Error	
DSP	Proxy certificate has expired

Appendix Figure 9.3 End user workflow configuration checking

Details:

1. Configure

Hitting this button opens a new form:

- Only those parameters of a Workflow can be changed which have been selected as such by the developer of the Application. Technically the end-user sees the input parameters separated by lines:
- There is an obligatory label to identify the parameter before the input field by which the given input parameter can be changed or must be defined.
- There may be supplementary information hidden by a little "paper page" - icon in the line of the parameter. Clicking on the icon the information can be read.
- The label and the supplementary information is defined when the experienced user creates a Template and opens a configuration parameter for the end-user.
- As a result the end-user gets all changeable parameters of a complex Application (which may include any number of embedded workflows as well) in a single page, while the experienced user using the full capacity of the system must visit the proper places in the definition hierarchy to fetch the tools (Graph Editor, Job Property, Port Property configuration) to pinpoint the changeable/definable parameters through a proper "keyhole".

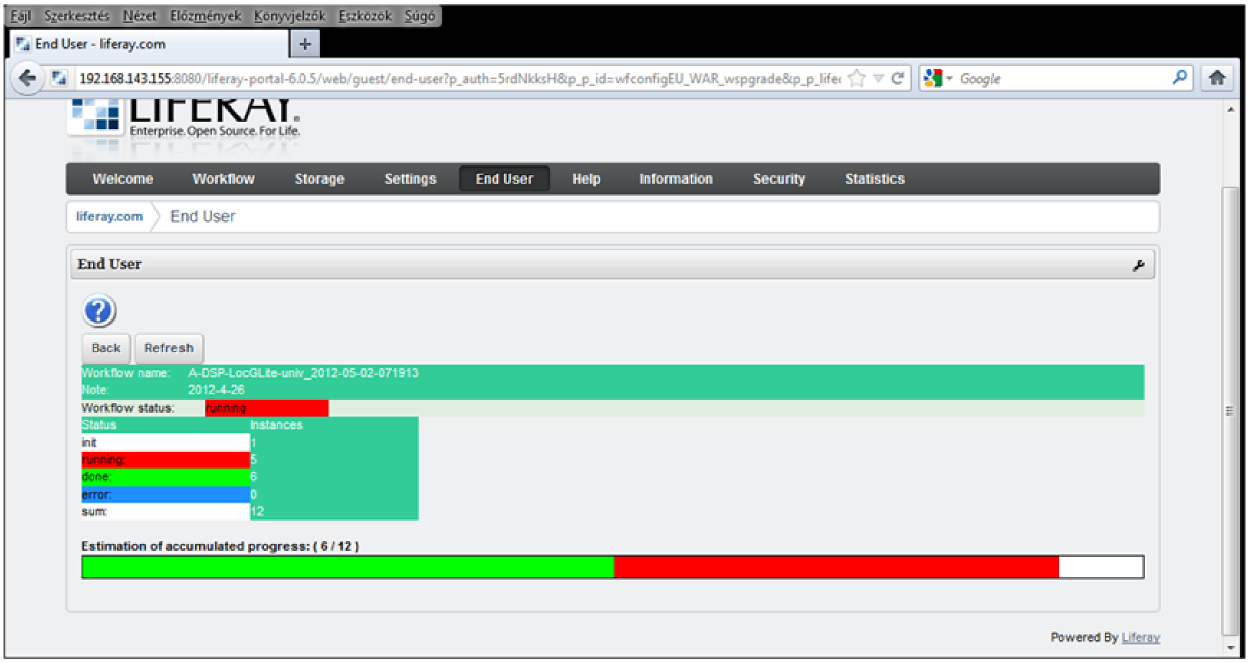
The type of an input field may be

- string,
- number,
- enumerated value selected by a radio button selector,
- or a file selected by a file browser.

The change have been done by the user must be confirmed by the *Save on Server* button.

2. Info

- The *Info* button helps to control the correctness of the Application.
- In the most common case the lack of a proxy certificate authorizing the user to submit the application can be read here.
- Using the Certificate tab the user can download the needed short time proxy certificates from the MyProxy server.
- Please note that the application may use several different destination environments (several grids and/or Virtual Organizations) and they may need different certificates or (certificate extensions) therefore the proxy certificates must be associated with the proper grid/VO.


Fájl Szerkesztés Nézet Előzmények Könyvjelzők Eszközök Súgó
End User - liferay.com
192.168.143.155:8080/liferay-portal-6.0.5/web/guest/end-user?p_auth=5rdNkksH&p_p_id=wfconfigEU_WAR_wspgrade&p_p_lifec
Google
LIFERAY.
Enterprise. Open Source. For Life.
Welcome
Workflow
Storage
Settings
End User
Help
Information
Security
Statistics
liferay.com
End User
End User
Back
Refresh
Powered By Liferay

Workflow name: A-DSP-LocGLite-univ_2012-05-02-071913

Note: 2012-4-26

Workflow status: running

Status	Instances
init	1
running:	5
done:	6
error:	0
sum:	12

Estimation of accumulated progress: (6 / 12)

Appendix Figure 9.4 Detailed view about end user workflow configuration status

3. Submission

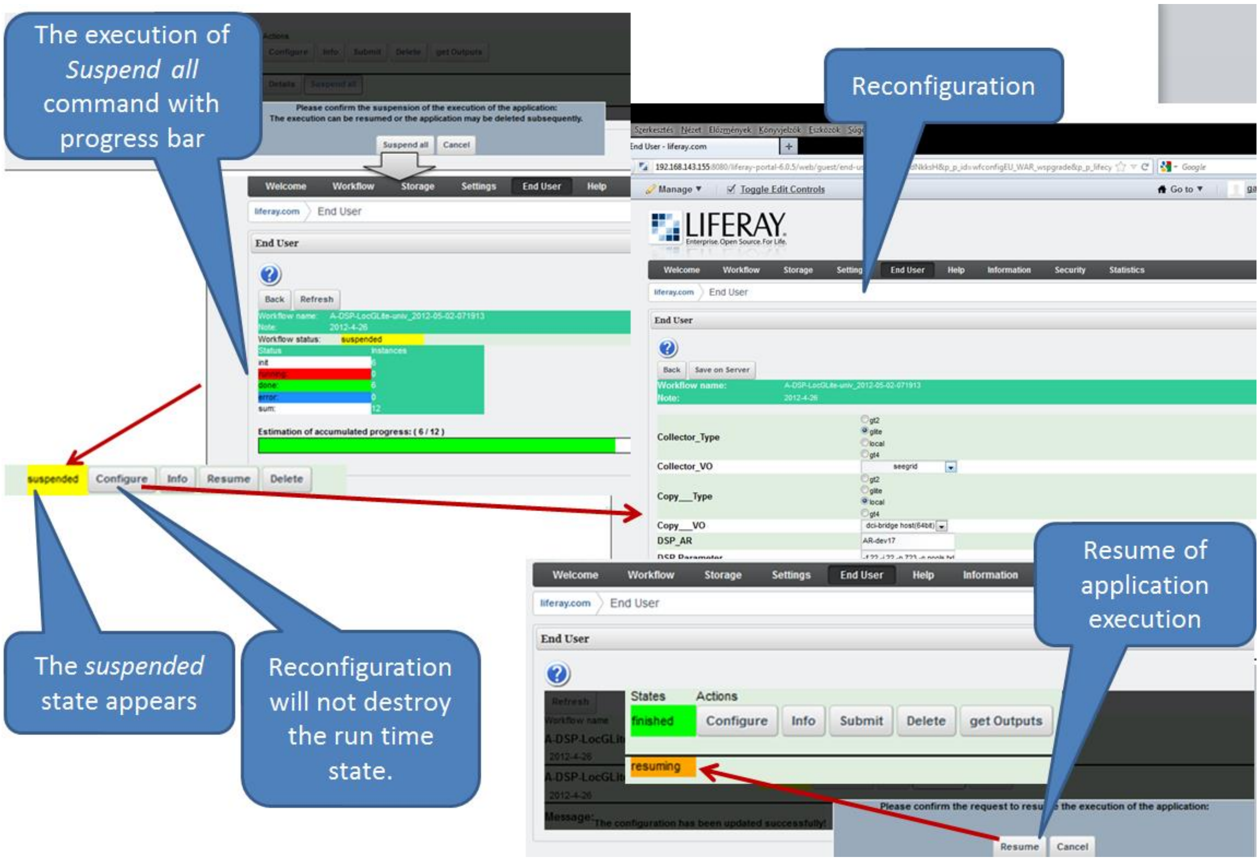
The *Submit* button serves the starting of the *Application*.

a) **States**: This button (synchronized by the application) has several states (and labels) and hitting the button the first time its new label will be *Suspend all*. Hitting the *Suspend all* button the application will be suspended, and the button will be labeled as *Resume* with the proper consequences of hitting it, or the user can select in this state the reappearing *Configuration* button to abort the submission indirectly (see Appendix Figure 42). The proper state of the submitted application is rendered graphically by a text message appearing in a little box whose background color is associated to the state.

   b) **Data**: One main lesson to learn here is the following: Other than in the case of the of the experienced user regime (*Workflow/Concrete Workflow* tab -> *Submit* button) there will be created just a single common instance of the Application (containing the outputs and the run time state of the workflow(s)) upon the submission of the Application. The consequence is that the user should save/remember the results (and/or inputs) of the submitted Application to prevent the overwriting of it before submitting the same Application the next time.
   c) **Notification**: Similar to the advanced user regime the end-user may receive e-mail notification about the termination/state change of the submitted application. However the prerequisite of the messaging is the proper setting the *Notify* tab.

4. **Fetching the results**: The *get Outputs* button appears upon the successful termination of the application. Hitting the button the file download mechanism of the applied internet browser will be opened by which the local output files supplied by the main workflow of the application can be downloaded. If the user is interested in a more detailed view of the results (inputs, circumstances) or just wants to archive the made experiment she can do it by downloading the application within the *Storage* tab selectable even in the end-user regime.

5. **Deleting the application**: The *Delete* button erases the application completely and therefore it must be handled with care. However a deleted application can be rebuilt from the repository.


The execution of *Suspend all* command with progress bar
Reconfiguration
Actions
Configure
Info
Submit
Delete
get Outputs
Details
Suspend all
Suspend all
Cancel
Welcome
Workflow
Storage
Settings
End User
Help
liferay.com
End User
Back
Refresh
Workflow status: suspended
Estimation of accumulated progress: (6 / 12)
suspended
Configure
Info
Resume
Delete
LIFERAY
Back
Save on Server
Collector_Type
Collector_VO
Copy__Type
Copy__VO
DSP_AR
The *suspended* state appears
Reconfiguration will not destroy the run time state.
Resume of application execution
States
Actions
finished
resuming
Resume
Cancel

Please confirm the suspension of the execution of the application:
The execution can be resumed or the application may be deleted subsequently.

Message: The configuration has been updated successfully!

Please confirm the request to resu… the execution of the application:

Appendix Figure 9.5 The Suspend function of End User menu: in this state the reconfiguration process don't destroy the run time state of job

10. The Certificates Menu

10.1 Introduction

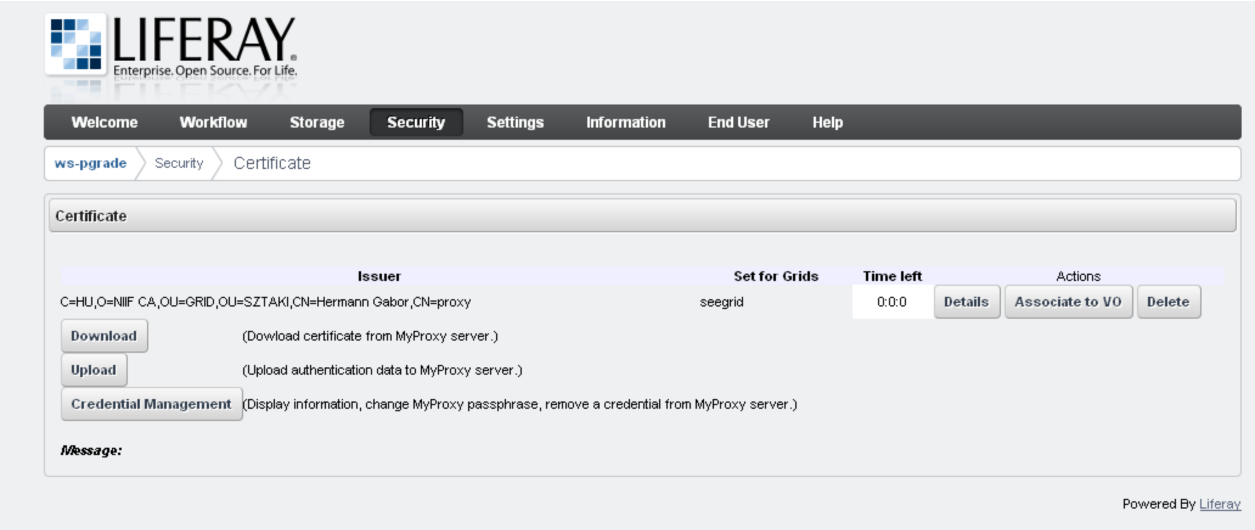
The users are identified and authorized to use the resources of the Grid by X.509 Certificates. The procurement procedure of the personal grid related certificates is out of the scope of this manual. Within the EGI infrastructure the resources of a given Virtual Organization are restricted for the members. The personal certificate is an unavoidable condition to obtain a VO membership. The procurement procedure of a VO membership is out of the scope of this manual.

10.1.1 Supporting VO-s using MyProxy Servers

Most of the VO-s of the EGI support the VOMS management. It means the VO specific extension of the Certificate. In this way a user may be the member of more than one VO in one time. Former this was prohibited, because the sites served more than one VO could not determine the VO membership of the certificate's owner, which caused problems – among others - in accounting, and in using the Storage Elements, maintained by the given site. For safety reason the jobs are not submitted to a resource in the company of a long term user certificate (which has a one year long validity expiration), but by using a substituting short term, so called proxy certificate (with a validity expiration time, limited in 100 hours), which is issued by a secure - so called MyProxy - Server playing the role of a Certificate Authority, against the submission of the long term user certificate. The application of the VOMS and MyProxy server solves - in principle - the problem of submitting jobs running longer than the expiration time of the proxy certificates: If the user declares the URL of the MyProxy server in the JDL of the job, then the infrastructure of the resource is able to reach the MyProxy server and it permits the user to generate a fresh, new, valid proxy certificate. The running of jobs can be continued with the recently created valid proxy certificate. Therefore, it is important to use such a MyProxy server which is reachable and trusted by the given resource. To fulfill this requirement the Virtual Organizations maintain own MyProxy servers.

The certificate menu (*Certificate* tab) helps the user

- to create a certificate account on the requested MyProxy server which stores the long term certificate of the user; and
- by referencing this account - to generate proxy certificates of the required expiration time with the intention to use them in the requested resources (VO-s).



Issuer	Set for Grids	Time left	Actions
C=HU,O=NIIF CA,OU=GRID,OU=SZTAKI,CN=Hermann Gabor,CN=proxy	seegrid	0:0:0	Details Associate to VO Delete

Download (Dowload certificate from MyProxy server.)

Upload (Upload authentication data to MyProxy server.)

Credential Management (Display information, change MyProxy passphrase, remove a credential from MyProxy server.)

Message:

Appendix Figure 10.1 The Certificate Menu - main view

Shortly speaking, this menu supplies the base functionalities of a MyProxy server in a user friendly way. The tab Certificate lists the existing proxy-certificates of the user with their expiration time (column Time left), with the current resource bindings (column Set for Grids) and with associated control buttons:

- *Details*: shows the details of the proxy (owner, original issuer, issuer of the proxy, etc.)
- *Associate to VO*: Opens an option window to associate an additional resource (VO) to the given proxy.
- The offered list of Virtual Organizations is taken from the *Settings* list
- *Delete*: deletes the given proxy.

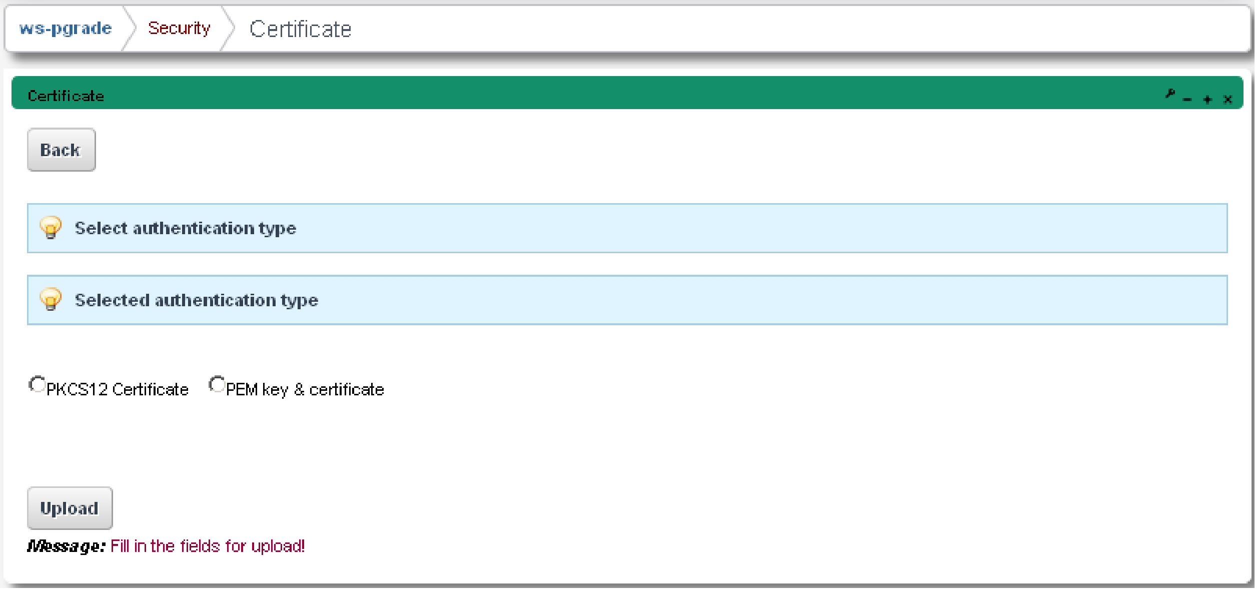
Further, the page features the following general operation buttons:

- *Upload* button: a new certificate account can be created. (See 10.2.1 Creating an account on the MyProxy Server).
- *Download* button: a new short term proxy certificate can be created and downloaded on the server, from where upon subsequent job submissions the system automatically attaches the proxy to the proper job. (See 10.2.3 Creating a proxy certificate).
- *Credential Management* button: the created certificate accounts can be deleted and the belonging passwords modified (See 10.2.4 Credential Management).

10.2 Upload

The functionality of the upload has been partly extended and partly reconsidered (in case of grids, which use SAML assertions) in the new versions (from version 3.4) of the gUSE/WS-PGRADE portal.

Upload remained the main mechanism to create the long term user accounts on the MyProxy servers on the base of presented personal user certificates, and the uploading mechanism permits in this new version the usage of the **PKCS12** format of the presented user certificates beyond the traditional **PEM** representation.


ws-pgrade
Security
Certificate
Certificate
Back
Select authentication type
Selected authentication type
○PKCS12 Certificate
○PEM key & certificate
Upload

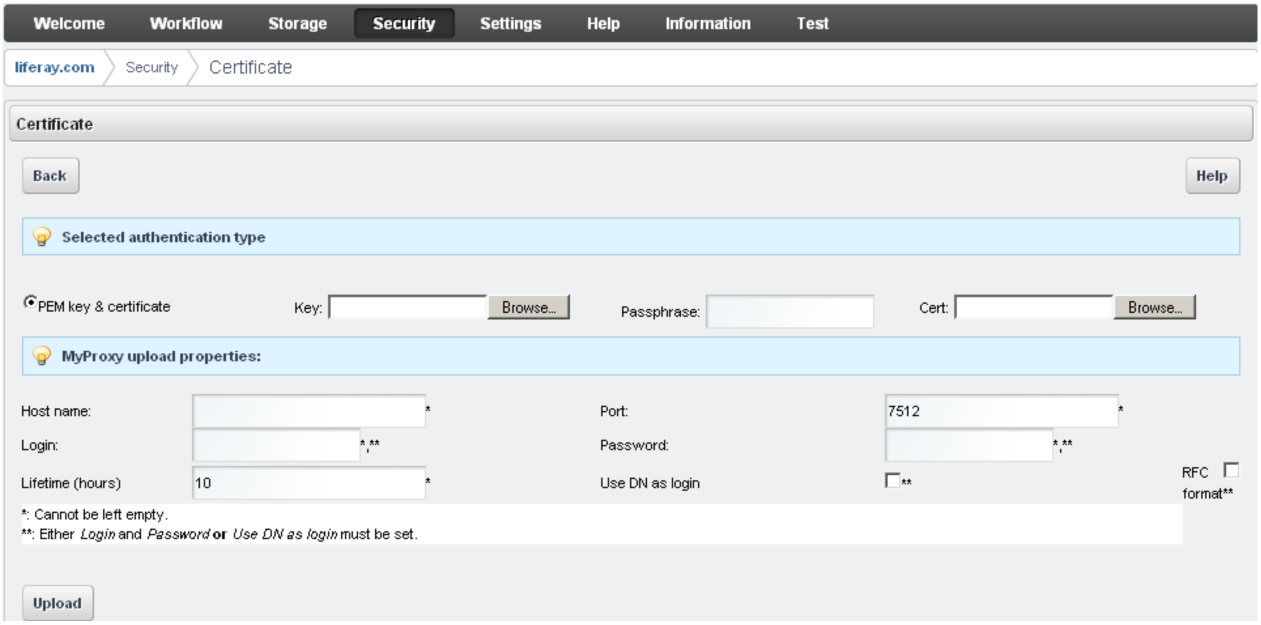
Message: Fill in the fields for upload!

Appendix Figure 10.2 Upload

10.2.1 Creating a user account on the My Proxy server

A user account can be created on the MyProxy Server by presenting either a single PKCS12 format file or the two PEM format files of a long term user certificate.

10.2.1.1 MyProxy account creation by presenting PEM files


Welcome
Workflow
Storage
Security
Settings
Help
Information
Test
liferay.com
Security
Certificate
Certificate
Back
Help
Selected authentication type
● PEM key & certificate
Key:
Browse...
Passphrase:
Cert:
Browse...
MyProxy upload properties:

Host name: *
Port: 7512 *
Login: *,**
Password: *,**
Lifetime (hours) 10 *
Use DN as login ☐**
RFC format** ☐

*: Cannot be left empty.
**: Either *Login* and *Password* or *Use DN as login* must be set.

Upload

Figure 10.2.1.1 Creation a My Proxy Account by presenting PEM files

First, the user must present the long term, grid related user certificate in the twin PEM file format, where the *userkey.pem* file contains the password protected secrete key, and the *usercert.pem* file that contains the CA signed public key of the certificate. The interactive system requests in the following subsequent steps:

1. the file "userkey.pem" (Key field),
2. the associated password (Passphrase: field)
3. the file "usercert.pem" (Cert field).

Notes:

For the vigilant reader it may be annoying that the 10.2.1.1 operation is performed not on the user’s desktop (we fill forms instead of using a trusted applets) therefore the file *userkey.pem* - against general security convention- travels through the net. However, the upload operation can be executed only if the whole portal is accessed by the secure socket connection (https://...)

Please remember, that a user at least once in a year - after obtaining the long term personal certificate - must execute the upload operation in the general case, and if he/she intends to submit long running jobs, then he/she must create the special account as well.

The certificate account can be stored in two different formats in the MyProxy Server: The GSI is the traditional default format. However some grids - for example the UNICORE - accepts only the RFC format. The checkbox RFC supports this form of storage.

10.2.1.1.1 General case of MyProxy Upload

After the presentation of the needed certificate files the MyProxy account can be defined – in the general case - by five input fields (See Figure 10.2.1.1):

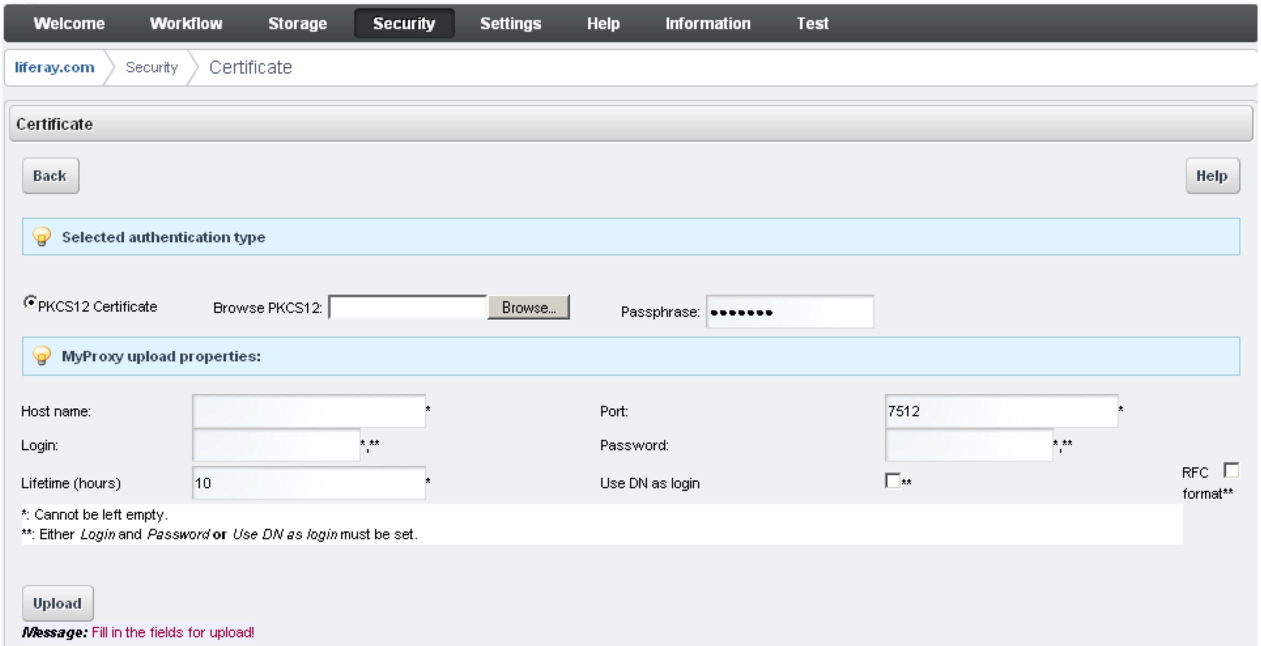
1. Host name is the URL of the MyProxy server, where the account is created
2. Port: is the port of the MyProxy server (the default port is 7512, if not defined otherwise)
3. Login: it is the freely selected name of the account. It must be unique!
4. Password: is a freely selected string, protecting the just created account
5. Lifetime(hours): Generic upper limit for the proxy certificates which will be subsequently generated using this account (See 10.2.3)

10.2.1.1.2 Special case for the automatic proxy renewal

In this special case, the fields Login and Password are not filled, but by marking the *Use DN as login* checkbox the distinguished name (which is readable from the certificate) will be used as Login name and a special account without password will be created. This account is used to the mentioned automatic proxy renewal, needed by a job wanting to survive the 100 hours absolute limit of proxy expiration time.

The special feature of this account is that it can be reached – other than the general account - only if a not expired proxy certificate exists, and then it generates a fresh one.

10.2.1.2 MyProxy account creation by presenting PKCS12 files


Welcome
Workflow
Storage
Security
Settings
Help
Information
Test
liferay.com
Security
Certificate
Certificate
Back
Help
Browse...
Upload

Selected authentication type

● PKCS12 Certificate Browse PKCS12: Passphrase: •••••••

MyProxy upload properties:

Host name: * Port: 7512 *
Login: *,** Password: *,**
Lifetime (hours) 10 * Use DN as login ☐** RFC format** ☐

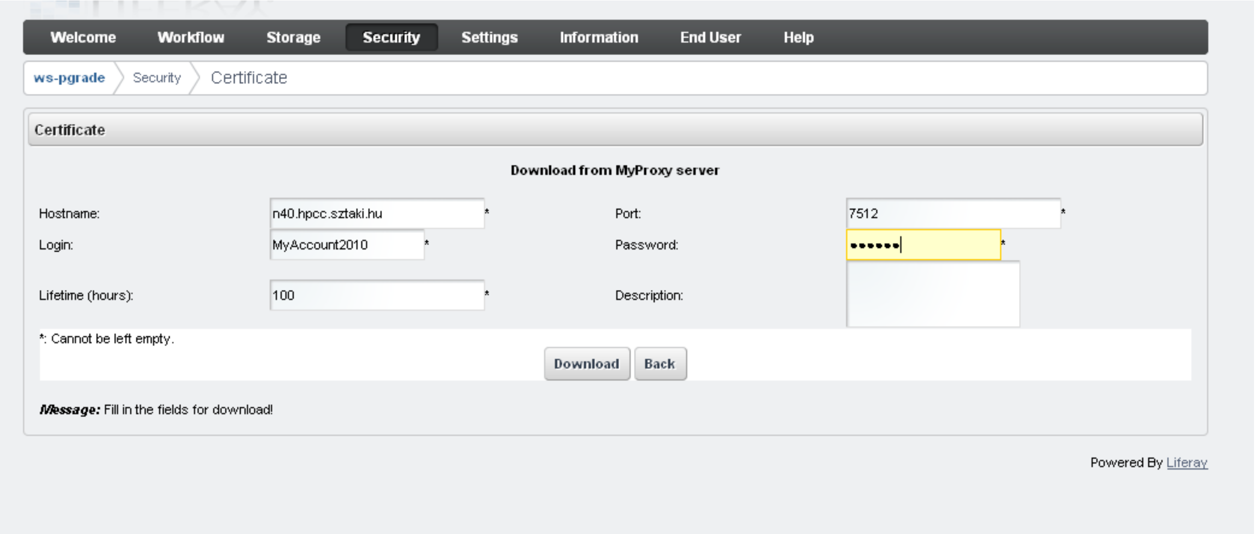
*: Cannot be left empty.
**: Either *Login* and *Password* or *Use DN as login* must be set.

Message: Fill in the fields for upload!

Appendix Figure 10.2.1.2 Creation a My Proxy Account by presenting a PKCS12

It is easy to see by the comparison with the Figure 10.2.1.1 belonging to the PEM case that only difference is that the user must present just a single PKCS12 format file with it passphrase instead of the two PEM files representing the long term user certificate. In any other respect the mechanism described in 10.2.1.1 and 10.2.1.2 perform the same job.

10.3 Creating a Proxy Certificate


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Security
Certificate
Certificate
Download
Back
Powered By Liferay

Download from MyProxy server

Hostname: n40.hpcc.sztaki.hu * Port: 7512 *
Login: MyAccount2010 * Password: •••••• *
Lifetime (hours): 100 * Description:

*: Cannot be left empty.

Message: Fill in the fields for download!

Appendix Figure 10.3 Certificate menu – Download a proxy certificate

Creating and downloading (from the MyProxy Server to the Portal Server) a short term proxy certificate is an "inverse" of the upload operation (See 10.2.2).

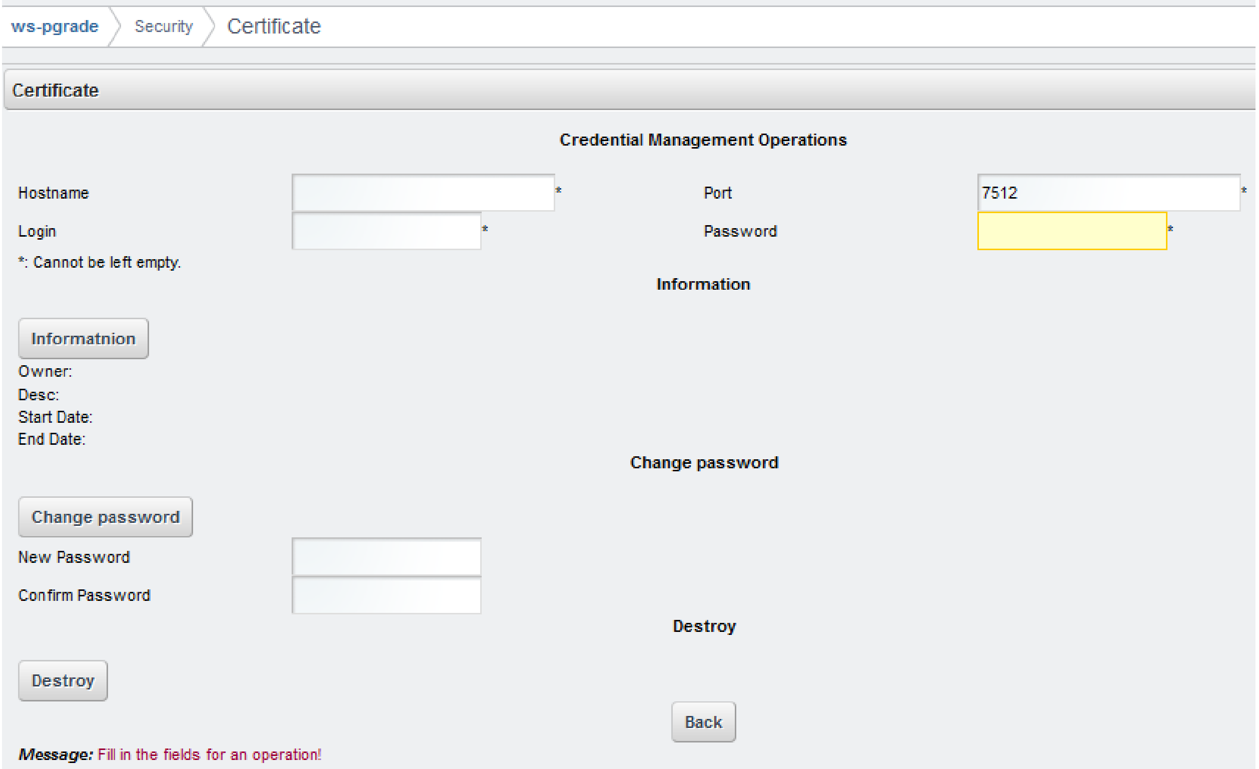
The same fields as in 10.2.1 must be filled to access the account.

Warning: The only exception is the Lifetime (hours): The real expiration time of the created and downloaded proxy certificate is the minimum of (*Upload.Lifetime, Download.Lifetime, 100 Hours*).

Please note that after a successful download the system immediately prompts the user to associate the created proxy certificates to an existing resource (which were created with the Settings menu). In one time a resource can be associated to just one certificate. This relation is certainly not true in the other direction: a single proxy certificate can have several resource bindings (as Figure 10.1 shows the settings of the user in column Set for Grids)

Pitfall: When you upload authentication data to MyProxy Server to use **gLite-based resources**, then you don't check the **RFC format** checkbox in the right corner of the Certificate window (see Appendix Fig. 10.2.1.2).

10.4 Credential Management



Hostname *
Port 7512 *
Login *
Password *
*: Cannot be left empty.

Owner:
Desc:
Start Date:
End Date:

New Password
Confirm Password

Message: Fill in the fields for an operation!

Appendix Figure 10.4 Certificate menu – Credential Management

With the help of the Credential management (through the Credential Management button on Certificate window) the user account storing the long term user certificate can be viewed and modified. This page is subdivided in four parts:

1. Identification part is similar to the one discussed in 10.2.1: The Proxy Server and the certificate account must be defined.
2. The content of Information will be updated by pressing the *Enter* button of the key pad terminating the input field of Password.
3. Information part returns the so called Distinguished Name (identifier) of the owner with the validity range of the certificate.
4. "Change password" part allows in a traditional way the replacement of the current password with a new one.
5. Pressing the *Destroy* button deletes the account from the MyProxy Server.

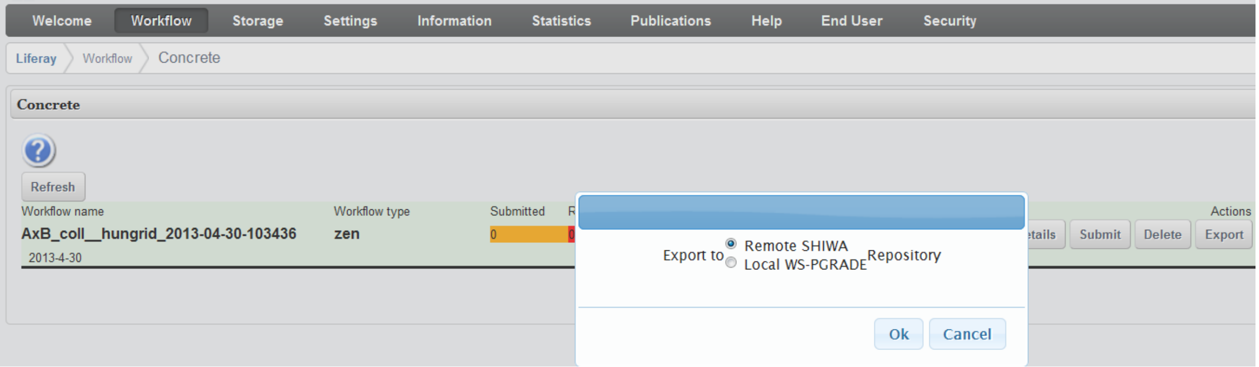
Note: the special account (see 10.2.2) might have been established using the Distinguished Name as the account name may not be handled by the Credential Management. The reason is that there is no need to do that:

This special account can be overwritten with a new one any time, so there is no need to destroy it or to change a non-existing password.

About the using of **robot permission** that used to identify applications instead of users, see chapter 20.

11. The Concrete/Export Menu

The **Concrete/Export** menu provides solution to export your workflows worth publishing. Workflows can be shared either in the **Local WS-PGRADE** community (i.e. they are usable among the users of the common portal server installation) or among the members of the SHIWA project community connected by the central SHIWA repository (by **Remote SHIWA** option) – see Appendix Figure 11.1.

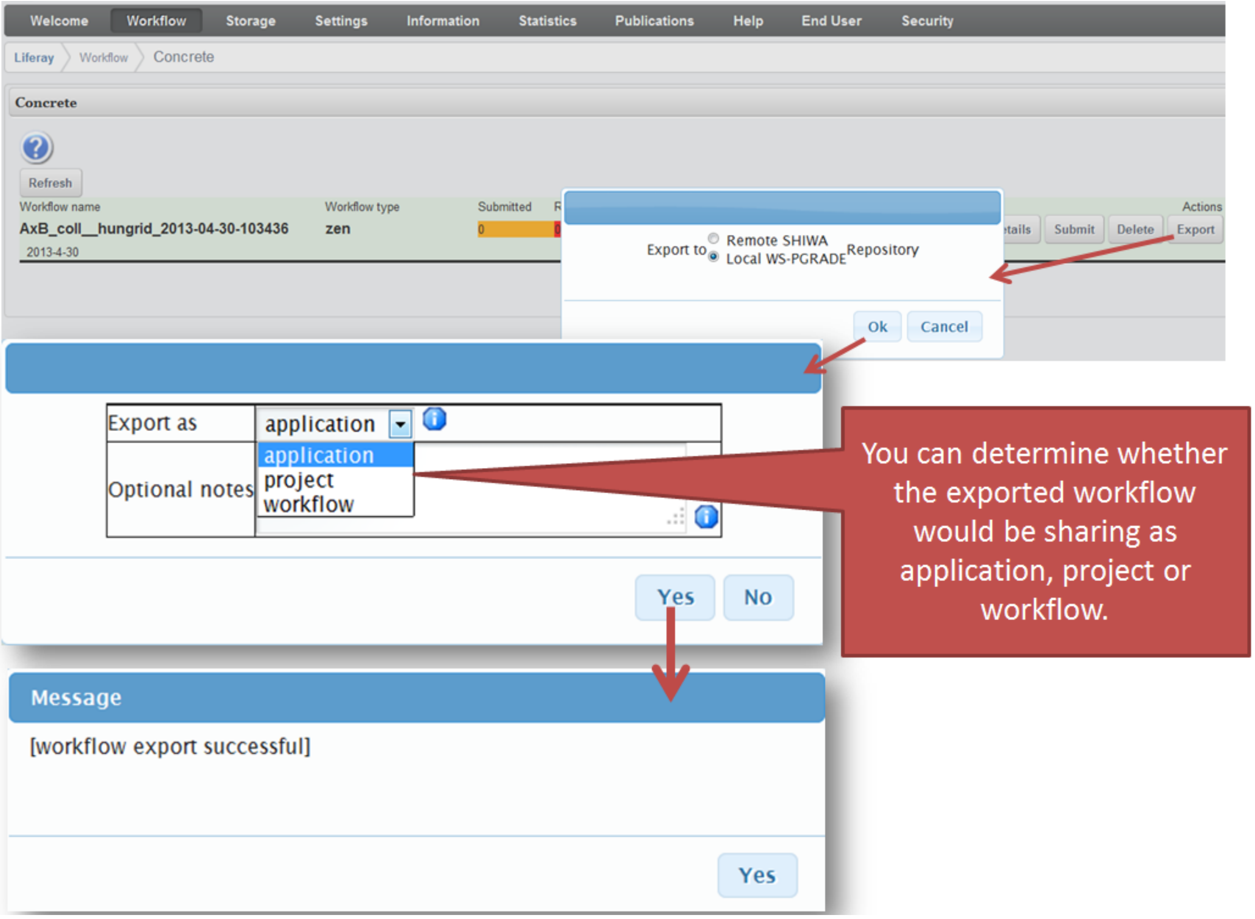

Welcome
Workflow
Storage
Settings
Information
Statistics
Publications
Help
End User
Security
Liferay
Workflow
Concrete
Concrete
Refresh
Workflow name
Workflow type
Submitted
Actions
AxB_coll__hungrid_2013-04-30-103436
zen
2013-4-30
0
Details
Submit
Delete
Export
Ok
Cancel

Export to ● Remote SHIWA ○ Local WS-PGRADE Repository

Appendix Figure 11.1 The first appearing dialog box of Export function controls the target community for workflow sharing. The dialog box appears after clicking on the Export button on the Workflow/Concrete window

1. **Workflow Export to Local WS-PGRADE Repository** (see Appendix Figure 11.2): In this case the export process contains only one step: the selection of the sharing type of your workflow. Three different kinds of objects can be distinguished and selected:
    - **Application** (default value): The term Application means the definition of a full tested Workflow (which involves the definition(s) of eventual embedded Workflows i.e. the definition includes the transitive closure of referenced workflows including graphs and templates taking part in the definition of them).
    - **Project:** The term Project means the "under construction" state of an Application i.e. it must not be full and tested however it contains the definition(s) of embedded workflow(s) if it is/they are available.
    - **Workflow:** The term Workflow involves the definition of its graph and may involve the definition of a Template if the workflow has been defined on the base of that template.

Warning: It must be remembered that all these objects have been created with optional verbose comments.


Welcome
Workflow
Storage
Settings
Information
Statistics
Publications
Help
End User
Security
Liferay
Workflow
Concrete
Concrete
Refresh
Workflow name
Workflow type
Submitted
Actions
tails
Submit
Delete
Export
Ok
Cancel
Yes
No
Message
Yes

AxB_coll__hungrid_2013-04-30-103436 zen 0
2013-4-30

Export to ○ Remote SHIWA Repository ● Local WS-PGRADE Repository

Export as: application
application
project
workflow
Optional notes

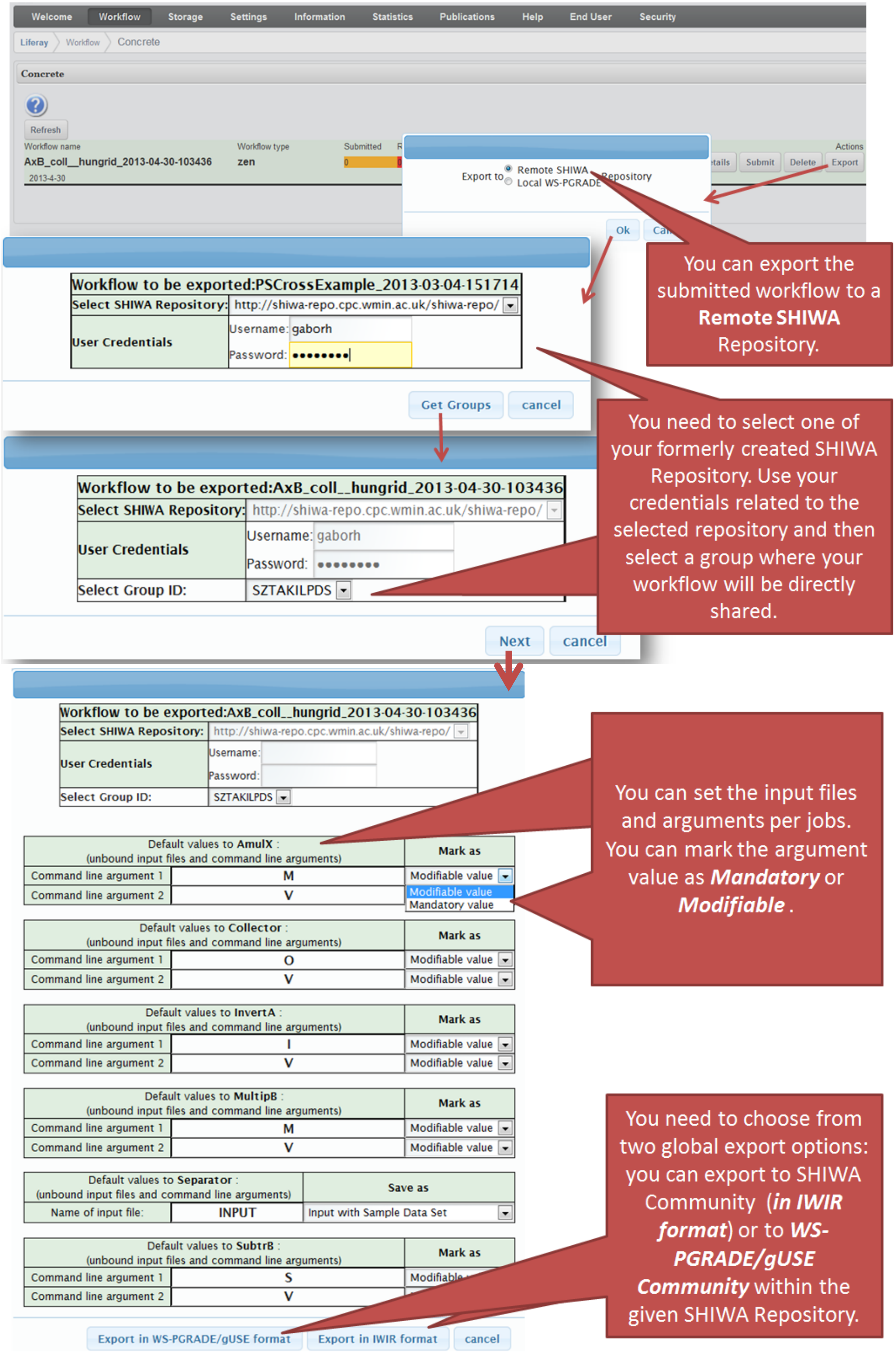
You can determine whether the exported workflow would be sharing as application, project or workflow.

[workflow export successful]

Appendix Figure 11.2 Export function 1: export your workflow to local WS-PGRADE Repository

2. **Export to Remote SHIWA Repository**: You can find the next two workflow export solutions within the **Export to SHIWA Repository** option. In order to select the corresponding solution you can just click either the **Export in IWIR format** or the **Export in WS-PGRADE/gUSE format** button at the end phase of the export setting process (see Appendix Figure 11.3) in WS-PGRADE.

   Let's see the similarities and the differences in the two solutions. The essential common point of this two export solutions is that the target place of remote exportation is a SHIWA Repository. If you want to share your workflow in the WS-PGRADE subset within the SHIWA Repository, click on **Export in WS-PGRADE/gUSE format** button. In this case your workflow doesn't come through an IWIR-based conversion, just put it a global WS-PGRADE-based workflow collection in a SHIWA repo. However, if you want to share your workflow to the whole repository that contains various workflows exported from various gateway systems within SHIWA community, click on **Export to IWIR format.**


Welcome
Workflow
Storage
Settings
Information
Statistics
Publications
Help
End User
Security
Liferay
Workflow
Concrete
Concrete
Refresh
Actions
Submit
Delete
Export
Ok
Get Groups
cancel
Next
cancel
Export in WS-PGRADE/gUSE format
Export in IWIR format
cancel

Workflow name	Workflow type	Submitted
AxB_coll__hungrid_2013-04-30-103436 2013-4-30	zen	0

Export to ● Remote SHIWA Repository ○ Local WS-PGRADE

You can export the submitted workflow to a **Remote SHIWA** Repository.

Workflow to be exported:PSCrossExample_2013-03-04-151714	
Select SHIWA Repository:	http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/
User Credentials	Username: gaborh Password: ••••••••

You need to select one of your formerly created SHIWA Repository. Use your credentials related to the selected repository and then select a group where your workflow will be directly shared.

Workflow to be exported:AxB_coll__hungrid_2013-04-30-103436	
Select SHIWA Repository:	http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/
User Credentials	Username: gaborh Password: ••••••••
Select Group ID:	SZTAKILPDS

Workflow to be exported:AxB_coll__hungrid_2013-04-30-103436	
Select SHIWA Repository:	http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/
User Credentials	Username: Password:
Select Group ID:	SZTAKILPDS

You can set the input files and arguments per jobs. You can mark the argument value as ***Mandatory*** or ***Modifiable*** .

Default values to **AmulX** : (unbound input files and command line arguments)		Mark as
Command line argument 1	M	Modifiable value Modifiable value Mandatory value
Command line argument 2	V	

Default values to **Collector** : (unbound input files and command line arguments)		Mark as
Command line argument 1	O	Modifiable value
Command line argument 2	V	Modifiable value

Default values to **InvertA** : (unbound input files and command line arguments)		Mark as
Command line argument 1	I	Modifiable value
Command line argument 2	V	Modifiable value

Default values to **MultipB** : (unbound input files and command line arguments)		Mark as
Command line argument 1	M	Modifiable value
Command line argument 2	V	Modifiable value

Default values to **Separator** : (unbound input files and command line arguments)		Save as
Name of input file:	INPUT	Input with Sample Data Set

Default values to **SubtrB** : (unbound input files and command line arguments)		Mark as
Command line argument 1	S	Modifiable
Command line argument 2	V	

You need to choose from two global export options: you can export to SHIWA Community (***in IWIR format***) or to ***WS-PGRADE/gUSE Community*** within the given SHIWA Repository.

Appendix Figure 11.3 Export function 2: export your workflow to global WS-PGRADE Repository

Warnings: In latter case (Export to IWIR format) you have to calculate some restrictions for workflows that come from the necessary IWIR-based conversion (the reason of these restrictions is to enable the convertibility and interoperability of various shared workflows[5]):

-The workflows must be executed before the export.
-The workflow instances are also exported by workflow export.
-The name of the workflow to be exported must contain only alphanumerical characters (You will get an error message when you want to export a workflow with another naming form).
-The export of embedded workflows is not supported.
-The export of workflows containing at least one job that has mixed dot- and cross product relation among its input ports is not supported.
-The remote mode of input file upload is not supported.
-The using of conditional port properties is not supported.
-The information about the resource settings (including the eventual user defined JDL settings) of workflow jobs will be lost during conversion to SHIWA repository environment.
-The defined values of PS (Parameter Sweep) input ports cardinality will be lost during conversion to SHIWA repository environment. It follows that workflows have jobs with free parametric input ports may not be exported.
-The export of a partly executed workflow (when not every job is terminated) is not supported.

Let's see the steps of exportation in case of remote export (see Appendix Figure 11.3):

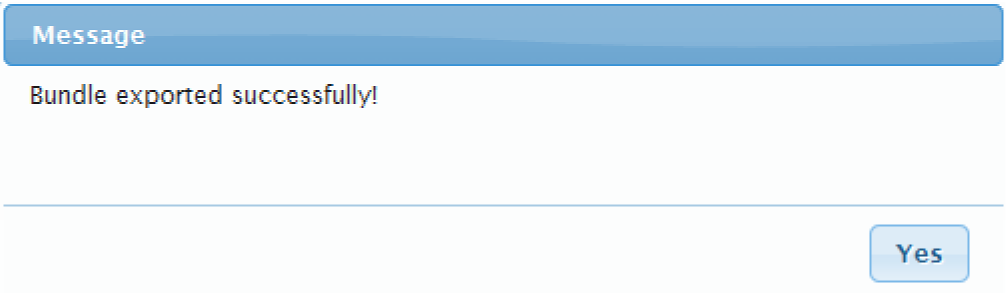
1. After you click **Export** button on **Concrete** page and select the **Export to Remote SHIWA Repository** option in the first appearing dialog box, you need to choose - after clicking on **Next** - a SHIWA repository URL and you need to give your valid authentication data to access the selected SHIWA repository. Click **Get Groups**.
2. Select one of your formerly created groups where you will share your workflow. Click **Next**.
3. In the last step you can add permissions to the formerly selected group and to other users in SHIWA community for defining and constraining the accessibility rights of your workflow.
    a. If you want to share your workflow only to WS-PGRADE community that uses WS-PGRADE-based workflows, click on **Export in WS-PGRADE/gUSE format** button
    b. If you want to share your workflows to a user community that uses other workflow management systems than WS-PGRADE, click on **Export in IWIR format** button (in this case you have to calculate on some rigorous restrictions mentioned above).

Note: the setting values in column **Mark as** haven't got any semantic influences to repository in case of **Export in WS-PGRADE/gUSE format.**

4. After that you will get a message ("Bundle exported successfully") about successful export the workflow bundle (bundle means workflows together with input files, dependencies and descriptions). (see Appendix Fig. 11.4.)

---

[5] The workflow sharing process for SHIWA Community involves a conversion into a code of a common language called IWIR (Interoperable Workflow Intermediate Representation). This constraints of the conversion cause the listed restrictions in workflow configuration.



Bundle exported successfully!

Appendix Figure 11.4 The result message after a successful export

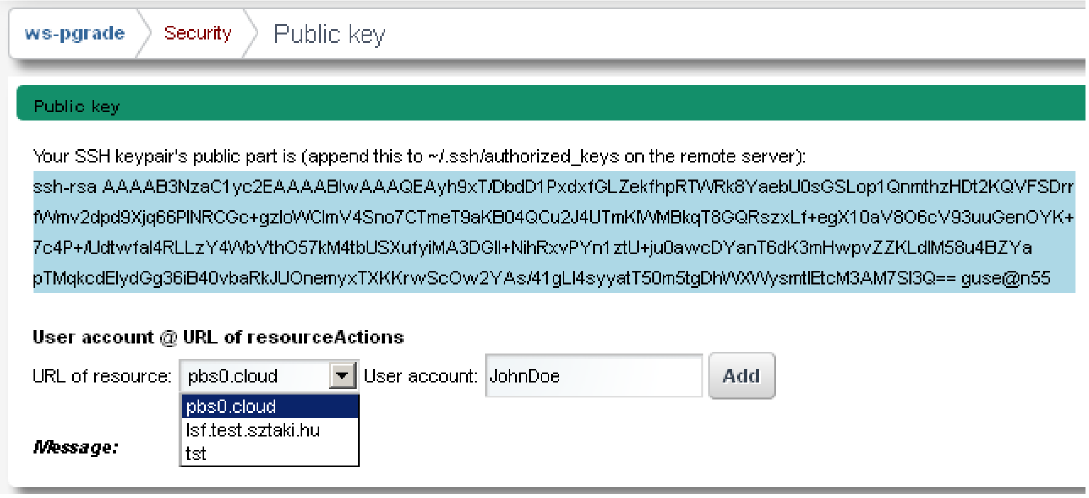
12. Public Key Menu

There are remote computational resources (**PBS**, **LSF, MOAB**[6]**,** and **SGE**[7] clusters) where the authorization and authentication of the user is not supported by the X.509 certificate standard. (About the PBS, LSF, SGE, and MOAB resources read the chapters 6.2.8, 6.2.9, and 6.2.20. The description of administration of LSF/PBS/SGE as well as MOAB can be found find in chapter 2.7 and in chapter 2.19 within *DCI Bridge Manual*.)

However, the traditional RSA public - private key mechanism can be used. The gUSE/WS-PGRADE infrastructure supports the user by the automatic generation of the needed RSA public - private key pair and by maintaining the SSL connection with those remote resources where the user has an account and the public key of the user is known. It follows that the user has three organizational duties in order to reach such remote computational resources by the WS-PGRADE - gUSE infrastructure:

1. An account must be gained on the proper (SGE, MOAB, PBS or LSF) remote resource.
2. The generated public key must be transferred to the named account.
3. The access data (account name, host, queue) of the remote resource must be registered in the gUSE/WS-PGRADE. The registered resource can be selected later during the configuration of a job.

It is obvious that the gUSE/WS-PGRADE gives only a passive support for the user that respecting the first two points: The menu shows the generated RSA Public key (blue area), which can be copied manually from the portal surface (see Appendix Fig. 12.1). The key generation happens in one time - together with generation of the user account on the WS-PGRADE portal.



Your SSH keypair's public part is (append this to ~/.ssh/authorized_keys on the remote server):

```
ssh-rsa AAAAB3NzaC1yc2EAAAABIwAAAQEAyh9xT/DbdD1PxdxfGLZekfhpRTWRk8YaebU0sGSLop1QnmthzHDt2KQVFSDrr
fWmv2dpd9Xjq66PINRCGc+gzloWClmV4Sno7CTmeT9aKB04QCu2J4UTmKMMBkqT8GQRszxLf+egX10aV8O6cV93uuGenOYK+
7c4P+/Udtwfal4RLLzY4WbVthO57kM4tbUSXufyiMA3DGII+NihRxvPYn1ztU+ju0awcDYanT6dK3mHwpvZZKLdlM58u4BZYa
pTMqkcdElydGg36iB40vbaRkJUOnemyxTXKKrwScOw2YAs/41gLl4syyatT50m5tgDhWXWysmtlEtcM3AM7SI3Q== guse@n55
```

User account @ URL of resourceActions

URL of resource: pbs0.cloud User account: JohnDoe

Message:

Appendix Figure 12.1 Public Key Menu

---

[6] The MOAB plugin development comes from the gUSE Community (exactly from Applied Bioinfomatics Group of Eberhard Karls University, Tübingen). If you have further questions, please send it to Luis de la Garza (delagarza@informatik.uni-tuebingen.de).

[7] The SGE plugin development comes from the gUSE Community (exactly from Optoelectronics and Visualisation Laboratory of Ruđer Bošković Institute, Zagreb). If you have further questions, please send it to Davor Davidovic (Davor.Davidovic@irb.hr).

A new remote PBS, LSF, MOAB or SGE resource access entry can be registered by filling the input fields:

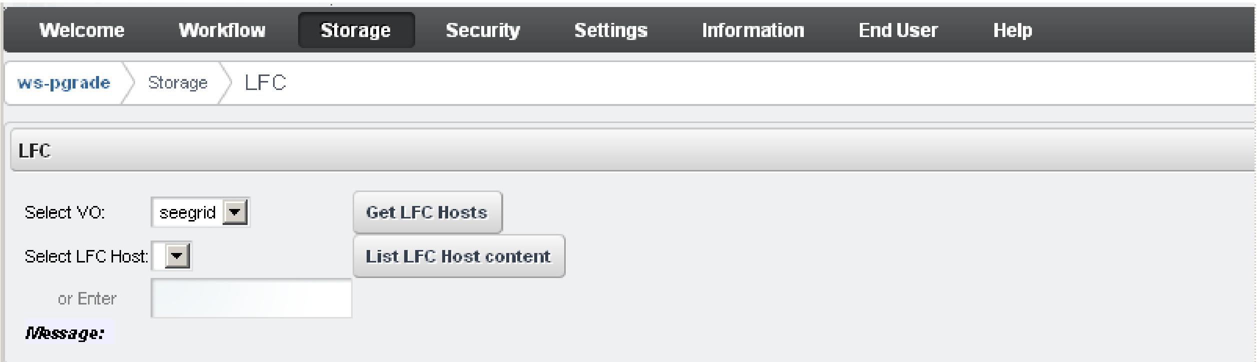
- User account: the user account on the remote cluster
- URL of resource: A selectable PBS resource defined by the DCI Bridge.

Confirmation is needed, and can be done by pressing the *Add* button. An existing access entry can be deleted by the associated Delete button. It is worth mentioning that the association of the resource and user account on the remote resource will be processed the following way:

1. An internal file will be generated which contains the user account name and the private key file.
2. The resource can be selected during Job configuration. See Figure Appendix Fig. 13 Part F
3. Upon job submit the file mentioned in (1) accompanies the job to the DCI-Bridge
4. So the DCI-Bridge playing the role of a client owning the secret key can communicate with the remote server (resource) logging in the named user account where the public key has been already set.

13. LFC Menu

File management menu provides **LCG File Catalogue (LFC)** operations and file management operations. Listing directories/files of an LFC name server, creating new directories, deleting or renaming directory/file entries, changing access modes of directory/file entries are the supported LFC interaction operations. Supported file management operations include uploading files to storage elements, downloading files from storage elements, listing replicas of files, replicating files between storage elements, deleting directories or files from storage elements, renaming, displaying their details (owner, group, last modification, access rights), and modifying the access rights.

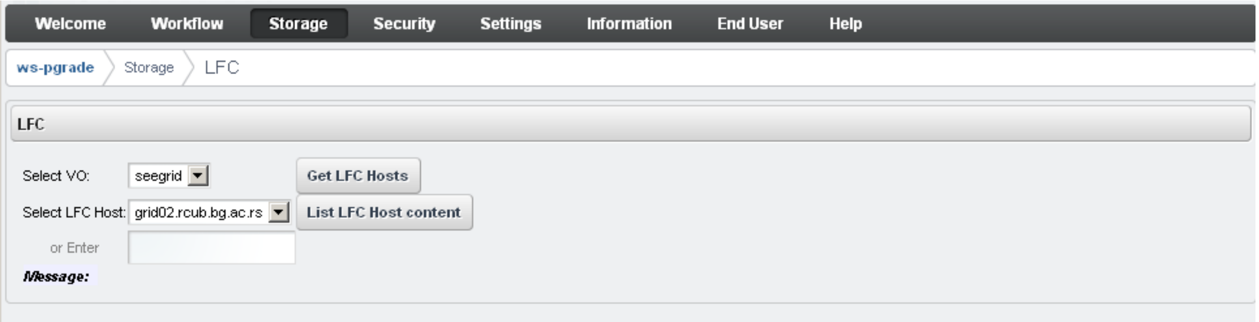

Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
seegrid
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
Message:

Appendix Figure 13.1 The LFC menu

To carry out file management operations, a user should download a short term proxy credential and map it to the virtual organization (VO) involved. The credential can also be mapped to a VO with broker support, for example "seegrid". For the credential that will be used, the portlet tries to find and use a credential mapped to the selected VO firstly.

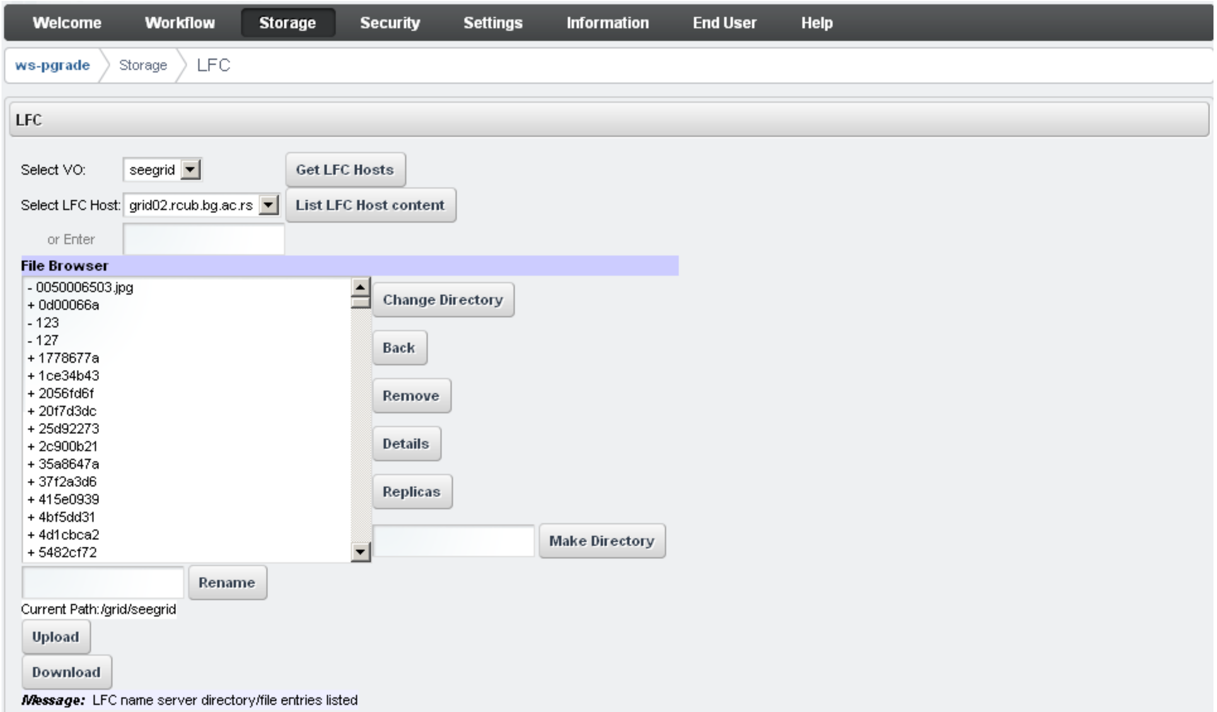
After creating a short term proxy and mapping it to a VO, following file management operations can be performed.

The user can select a VO using the combo boxes on the upper part of the file management portlet shown in Figure 13.1. LFC host name for that VO can be obtained by clicking the *Get LFC Hosts* button. As the BDII server of that VO, hostname and the port number provided in the *Settings* menu are used to set **LCG_GFAL_INFOSYS** variable. If these are not defined by the portal administrator for the selected VO, **LCG_GFAL_INFOSYS** variable is used as it is defined in the portal server's user interface (UI).


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
seegrid
Get LFC Hosts
Select LFC Host:
grid02.rcub.bg.ac.rs
List LFC Host content
or Enter
Message:

Appendix Figure 13.2 Browsing LFC Name Server Directory/File Entries

Directory/file entries of an LFC Host can be listed using the *List LFC Host content* button. Figure 13.3 shows the directory/file entries for the LFC host of *seegrid* VO.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Get LFC Hosts
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

Select VO: seegrid

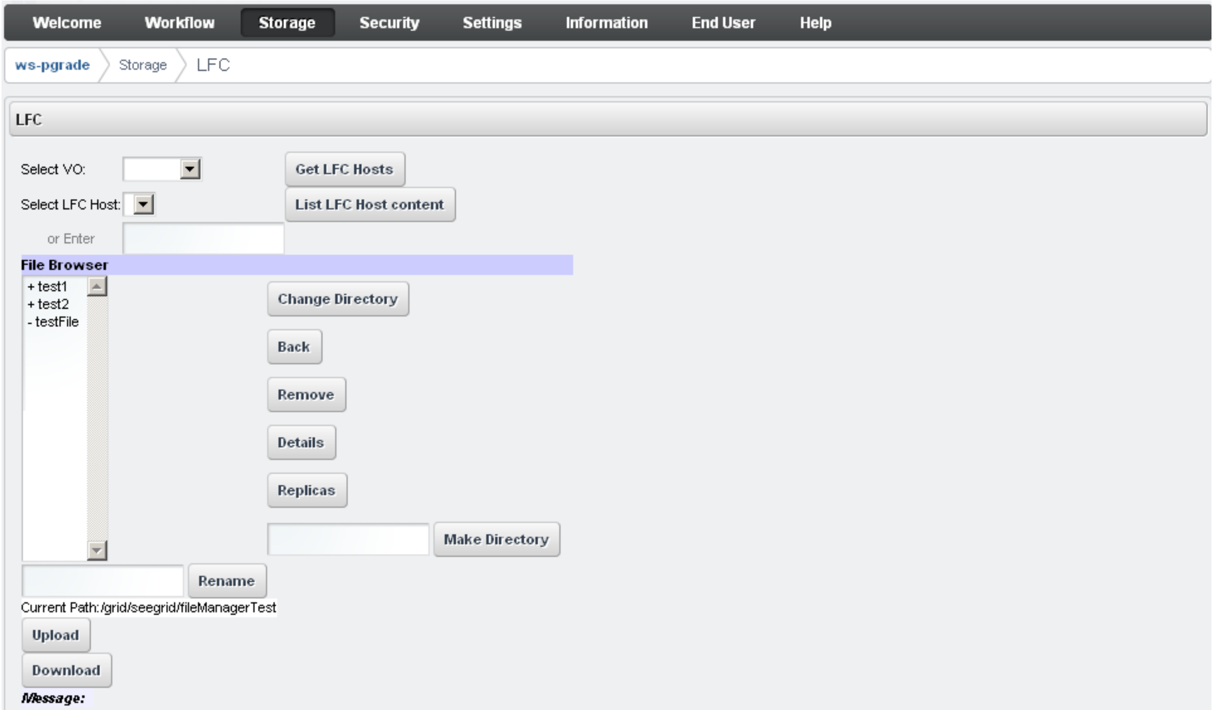
Select LFC Host: grid02.rcub.bg.ac.rs

- 0050006503.jpg
+ 0d00066a
- 123
- 127
+ 1778677a
+ 1ce34b43
+ 2056fd6f
+ 20f7d3dc
+ 25d92273
+ 2c900b21
+ 35a8647a
+ 37f2a3d6
+ 415e0939
+ 4bf5dd31
+ 4d1cbca2
+ 5482cf72

Current Path:/grid/seegrid

Message: LFC name server directory/file entries listed

Appendix Figure 13.3 On the file browser, directories are shown starting with a "+", and files are with a "-" sign.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Select LFC Host:
Get LFC Hosts
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

+ test1
+ test2
- testFile

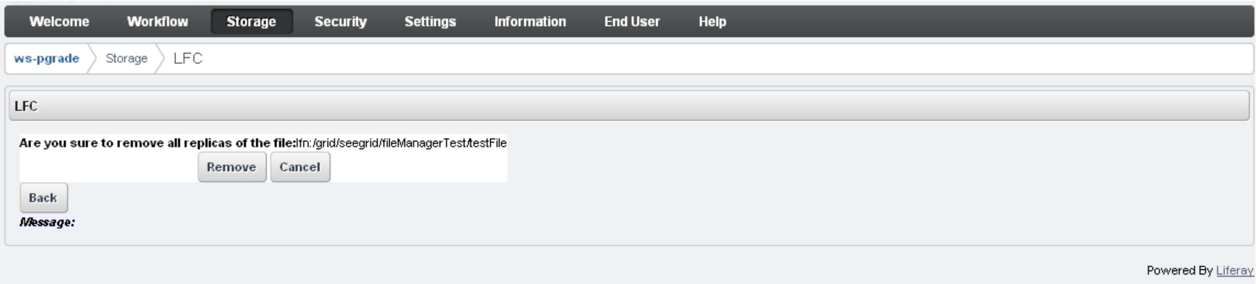
Current Path:/grid/seegrid/fileManagerTest

Message:

Appendix Figure 13.4 The *Back* button can be used to go back to the listing of the upper directory

After selecting a directory and clicking the *Change Directory* button, the user can list the contents of that directory. Contents of the */grid/seegrid/fileManagerTest* directory are listed as described and shown in Figure 13.4.

Removing a file/directory item: by selecting an item on the browser and clicking the *Remove* button, the user is directed to another page for the acknowledgement of the removal operation. This page is shown in Figure 13.5 for a file item.



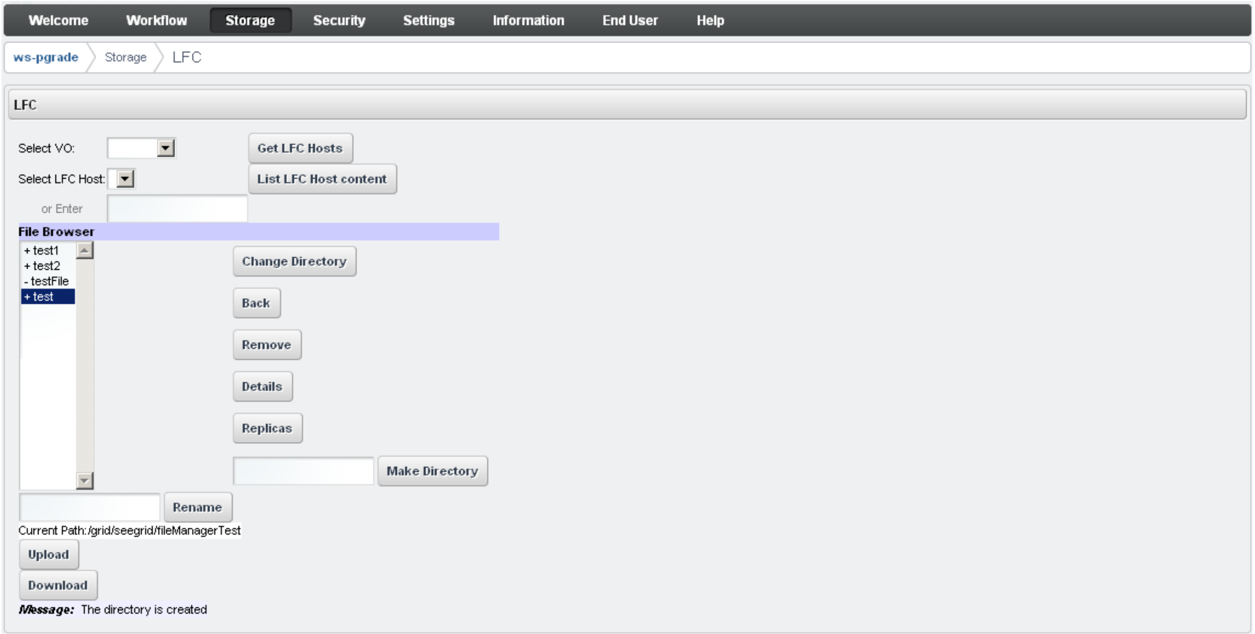
Are you sure to remove all replicas of the file:lfn:/grid/seegrid/fileManagerTest/testFile

Appendix Figure 13.5 Removing File/Directory

For files, all the replicas of that file are removed from storage elements, and LFN of that file is removed from LFC. For directory items, if the directory is empty, the directory is removed from LFC. If the directory is not empty, this operation removes all the replicas and LFN of all the files under the selected directory. The non-empty directories under the selected directory are not removed in a recursive way. The directory itself is removed from the LFC if it is finally empty.

Creating a Directory: The user can create a new directory using the *Make Directory* button on figure 13.3. The new directory will be created under the currently listed directory.

For example, to create a directory named *test* under */grid/seegrid/fileManagerTest*, the contents of */grid/seegrid/fileManagerTest* should be listed first. The name of the directory to be created should be provided through the text box next to *Make Directory* button. Then clicking on *Make Directory* button creates the new directory as shown in Figure 13.6.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

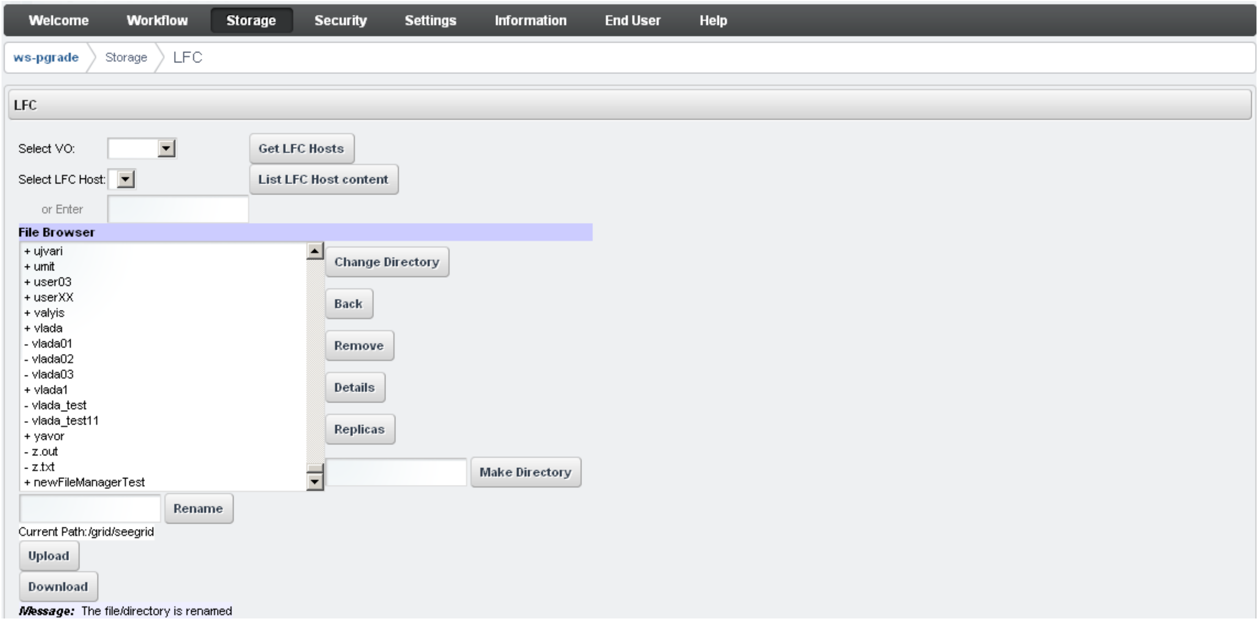
+ test1
+ test2
- testFile
+ test

Current Path:/grid/seegrid/fileManagerTest

Message: The directory is created

Appendix Figure 13.6

A file/directory item can be renamed using the *Rename* button on Figure 13.3. The item to be renamed should be selected and the new name should be provided through the text box next to *Rename* button.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

+ ujvari
+ umit
+ user03
+ userXX
+ valyis
+ vlada
- vlada01
- vlada02
- vlada03
+ vlada1
- vlada_test
- vlada_test11
+ yavor
- z.out
- z.txt
+ newFileManagerTest

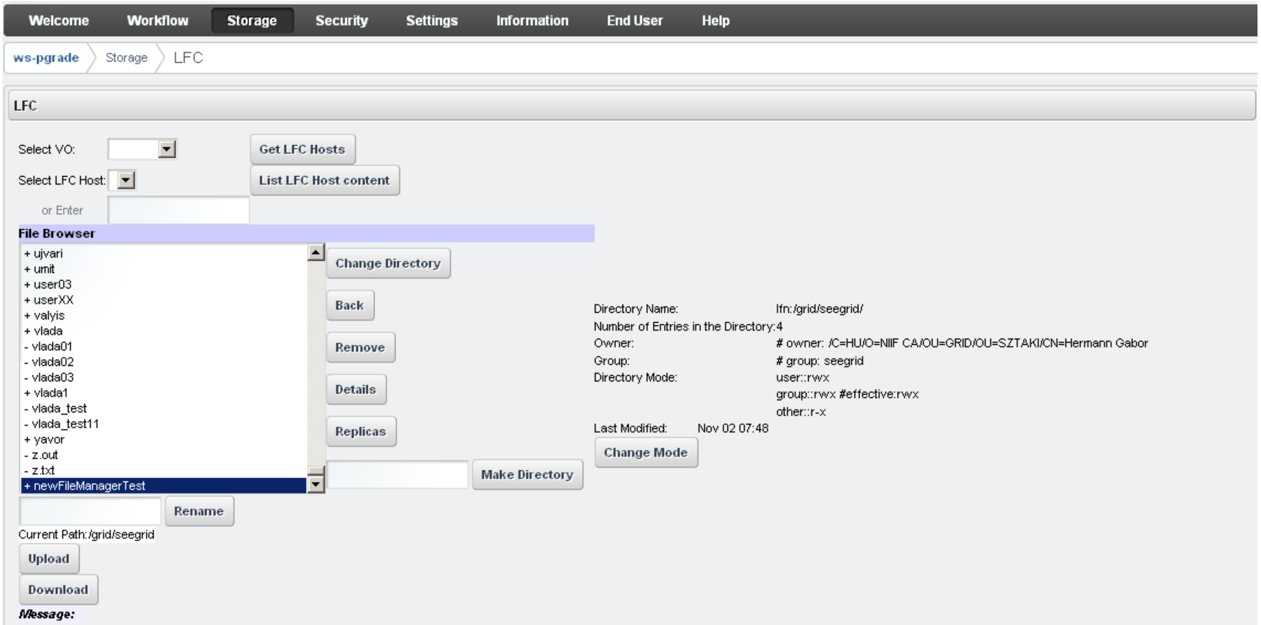
Current Path:/grid/seegrid

Message: The file/directory is renamed

Appendix Figure 13.7

On Figure 13.7, *fileManagerTest* directory under */grid/trgridb* is renamed as *newFileManagerTest*.

Getting detailed information for a file/directory Item: After selecting an item on the browser and clicking on *Details* button, further information about that item can be obtained. Figure 13.8 displays the result of this operation for the directory */grid/seegrid/newFileManagerTest* and Figure 13.9 displays the result of this operation for the file */grid/seegrid/newFileManagerTest/testFile*.

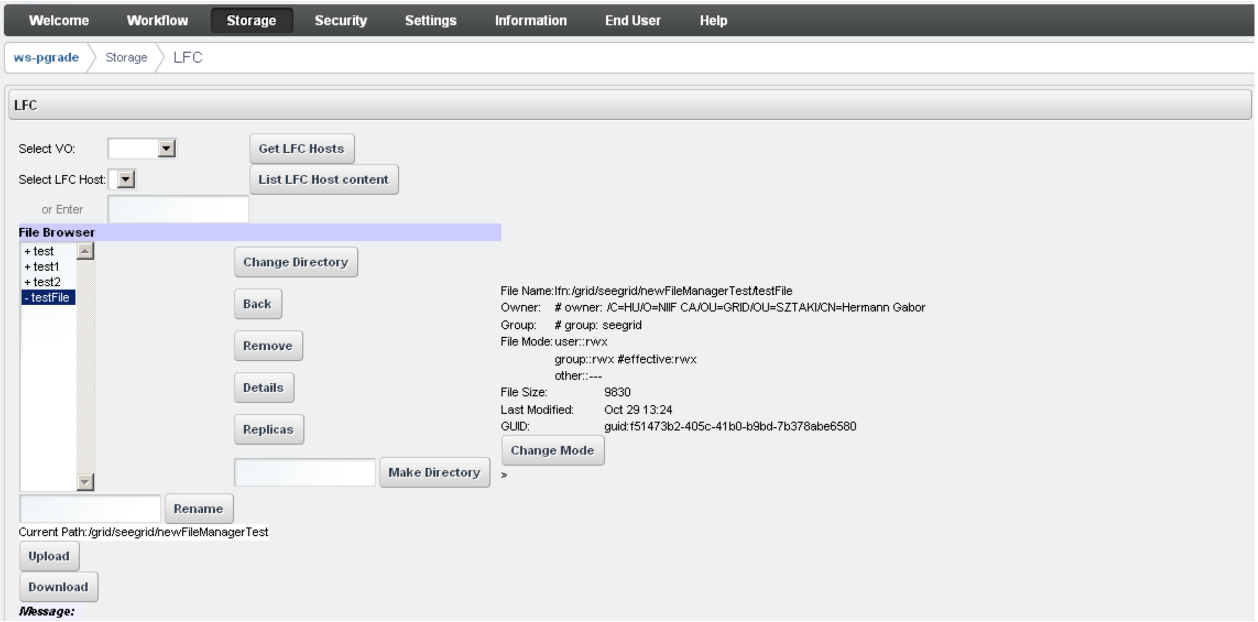

Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Change Mode
Rename
Upload
Download
Message:

+ ujvari
+ umit
+ user03
+ userXX
+ valyis
+ vlada
- vlada01
- vlada02
- vlada03
+ vlada1
- vlada_test
- vlada_test11
+ yavor
- z.out
- z.txt
+ newFileManagerTest

Current Path:/grid/seegrid

Directory Name: lfn:/grid/seegrid/
Number of Entries in the Directory:4
Owner: # owner: /C=HU/O=NIIF CA/OU=GRID/OU=SZTAKI/CN=Hermann Gabor
Group: # group: seegrid
Directory Mode: user::rwx
group::rwx #effective:rwx
other::r-x
Last Modified: Nov 02 07:48

Appendix Figure 13.8 Directory Details


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Change Mode
Rename
Upload
Download
Message:

+ test
+ test1
+ test2
- testFile

Current Path:/grid/seegrid/newFileManagerTest

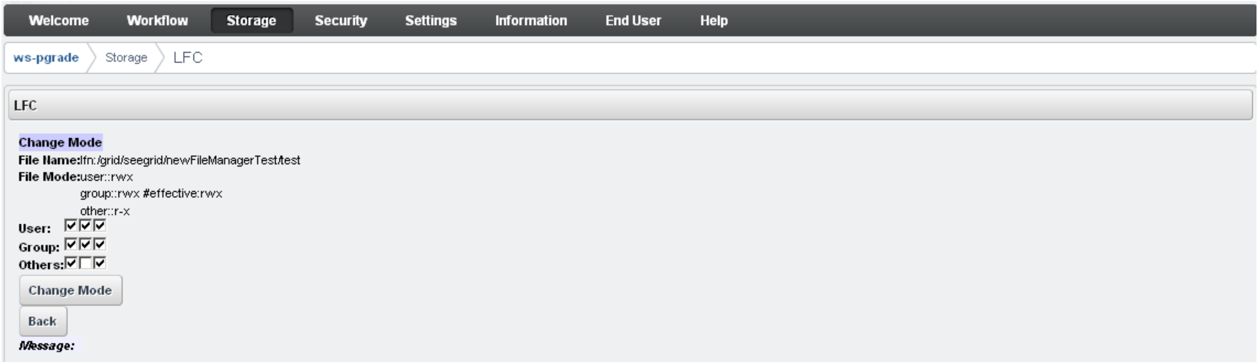
File Name:lfn:/grid/seegrid/newFileManagerTest/testFile
Owner: # owner: /C=HU/O=NIIF CA/OU=GRID/OU=SZTAKI/CN=Hermann Gabor
Group: # group: seegrid
File Mode: user::rwx
group::rwx #effective:rwx
other::---
File Size: 9830
Last Modified: Oct 29 13:24
GUID: guid:f51473b2-405c-41b0-b9bd-7b378abe6580

>

Appendix Figure 13.9 File Details

Changing Mode of a Directory/File Item: After displaying details for a directory/file item, "Change Mode" button is available as shown in Figure 13.8 and Figure 13.9. After clicking the "Change Mode" button, the user is directed to a new page and on this page, access modes for the directory/file item can be changed.

Figure 13.10 is obtained by listing the details for the directory "/grid/seegrid/newFileManagerTest/test" and clicking the *Change Mode* button afterwards.

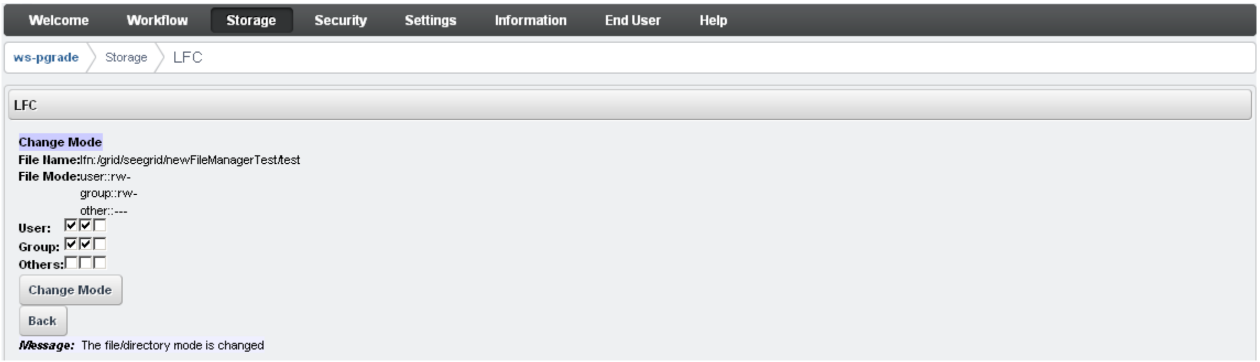

Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Change Mode
Change Mode
Back

File Name:lfn:/grid/seegrid/newFileManagerTest/test
File Mode:user::rwx
group::rwx #effective:rwx
other::r-x
User: ☑☑☑
Group: ☑☑☑
Others:☑☐☑
Message:

Appendix Figure 13.10 Change mode

To change the access modes for a directory/file, new access modes can be specified using the check boxes next to *User, Group* and *Others* labels. For example, to assign read and write permissions to user, the checkboxes labeled *Read* and *Write* next to *User* should be checked and others should be leaved unchecked. Access modes for the directory/file will be changed after clicking the *Change Mode* button.

On Figure 13.11, access modes of the directory are changed so that the user and the group both have read and write permissions and others have no permission.

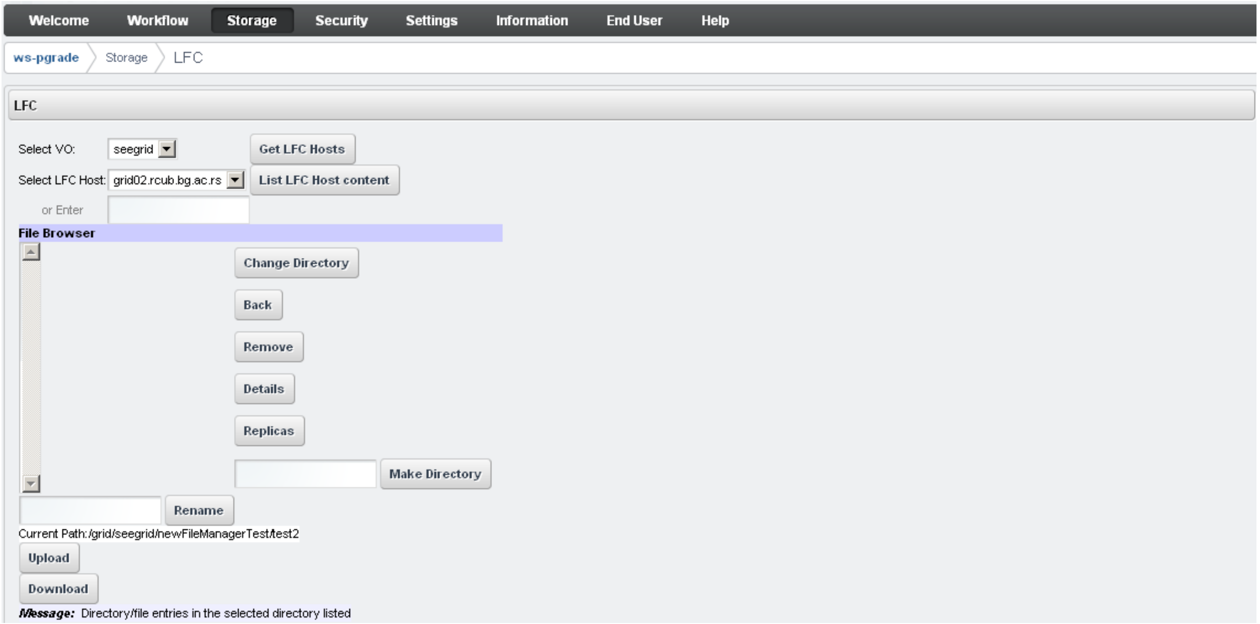

Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Change Mode
Change Mode
Back

File Name:lfn:/grid/seegrid/newFileManagerTest/test
File Mode:user::rw-
group::rw-
other::---
User: ☑☑☐
Group: ☑☑☐
Others:☐☐☐
Message: The file/directory mode is changed

Appendix Figure 13.11 Mode changed

Uploading a file to a Storage Element: *Upload* button on Figure 13.3 can be used to upload a file to a storage element. The file will be uploaded to the current directory. Therefore, to upload a file, the contents of the directory that the file is to be uploaded should be listed first.

For example, to upload a file under */grid/seegrid/newFileManagerTest/test2* directory, first, contents of that file is listed as shown in Figure 13.12 (the directory is currently empty).


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Get LFC Hosts
List LFC Host content
or Enter
File Browser
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

Select VO: seegrid

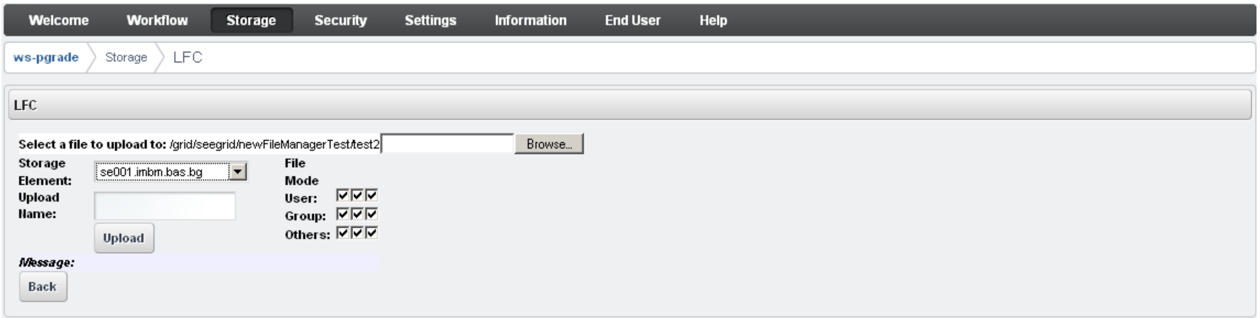
Select LFC Host: grid02.rcub.bg.ac.rs

Current Path: /grid/seegrid/newFileManagerTest/test2

Message: Directory/file entries in the selected directory listed

Appendix Figure 13.12 Directory before upload

Clicking on *Upload* button directs the user to a new page as displayed in Figure 13.13. On this page, storage elements for the VO that the user is currently working on are listed in the combo box next to *Storage Element* label. The storage element that the file is to be uploaded should be chosen from that combo box. The name of the new file on the LFC should be provided through the text box labeled *Upload Name*. And the file should be selected using the *Browse* button. The access modes for the file can be specified using the *File Mode* check boxes.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Browse...
Upload
Back

Select a file to upload to: /grid/seegrid/newFileManagerTest/test2

Storage Element: se001.imbm.bas.bg

Upload Name:

File Mode

User: ☑☑☑

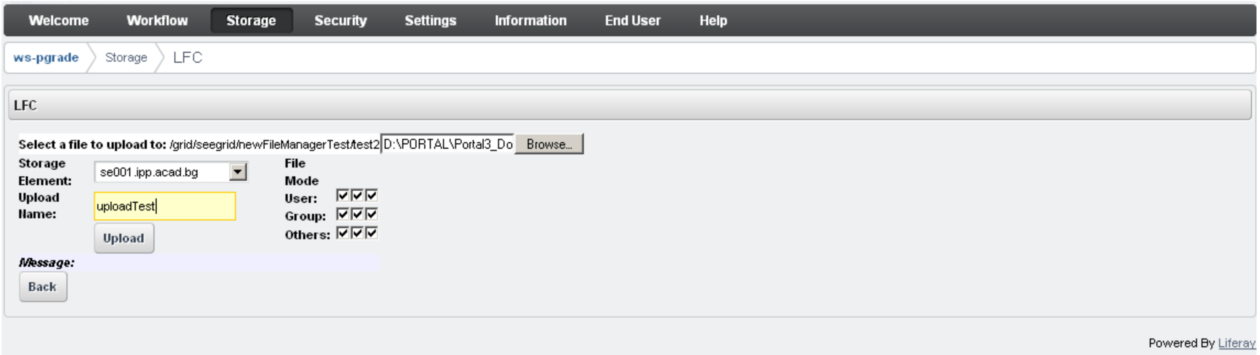
Group: ☑☑☑

Others: ☑☑☑

Message:

Appendix Figure 13.13 Upload page

On Figure 13.14, a new file is uploaded to the storage element *se001.ipp.acad.bg* with name *uploadTest* and the selected file access modes.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Browse...
Upload
Back
Powered By Liferay

Select a file to upload to: /grid/seegrid/newFileManagerTest/test2 D:\PORTAL\Portal3_Do

Storage Element: se001.ipp.acad.bg

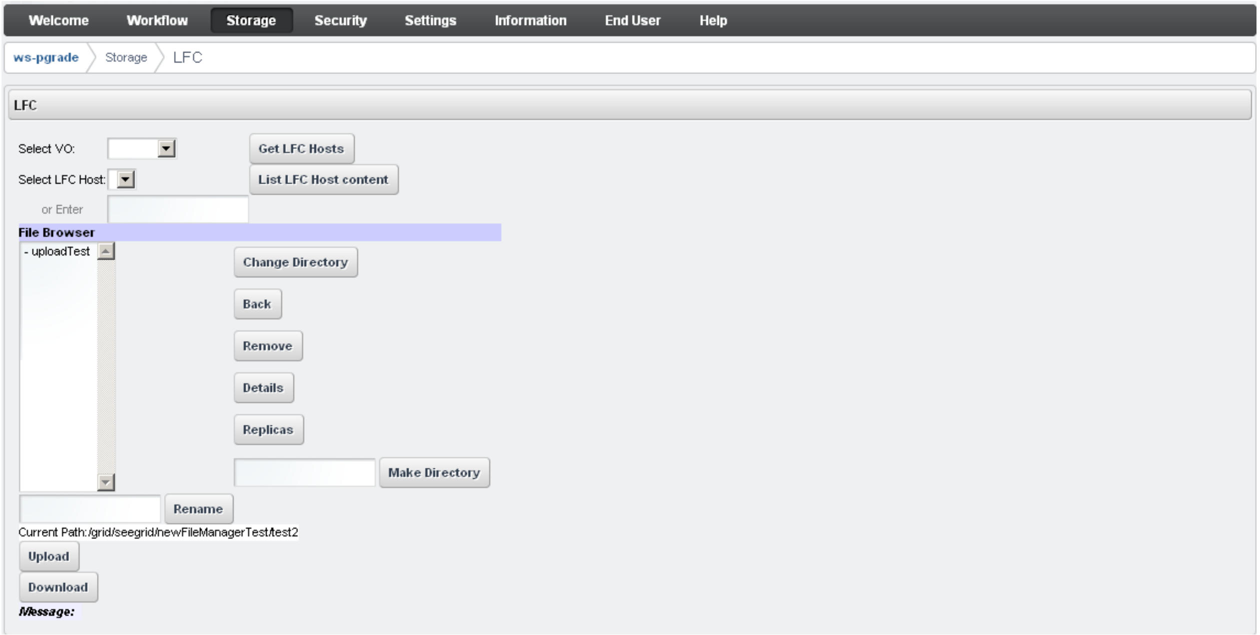
Upload Name: uploadTest

File Mode
User: ☑☑☑
Group: ☑☑☑
Others: ☑☑☑

Message:

Appendix Figure 13.14 Prepared Upload

Finally, the file can be listed under */grid/seegrid/newFileManagerTest/test2* as shown in Figure 13.15.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Get LFC Hosts
List LFC Host content
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

Select VO:

Select LFC Host:

or Enter

File Browser
- uploadTest

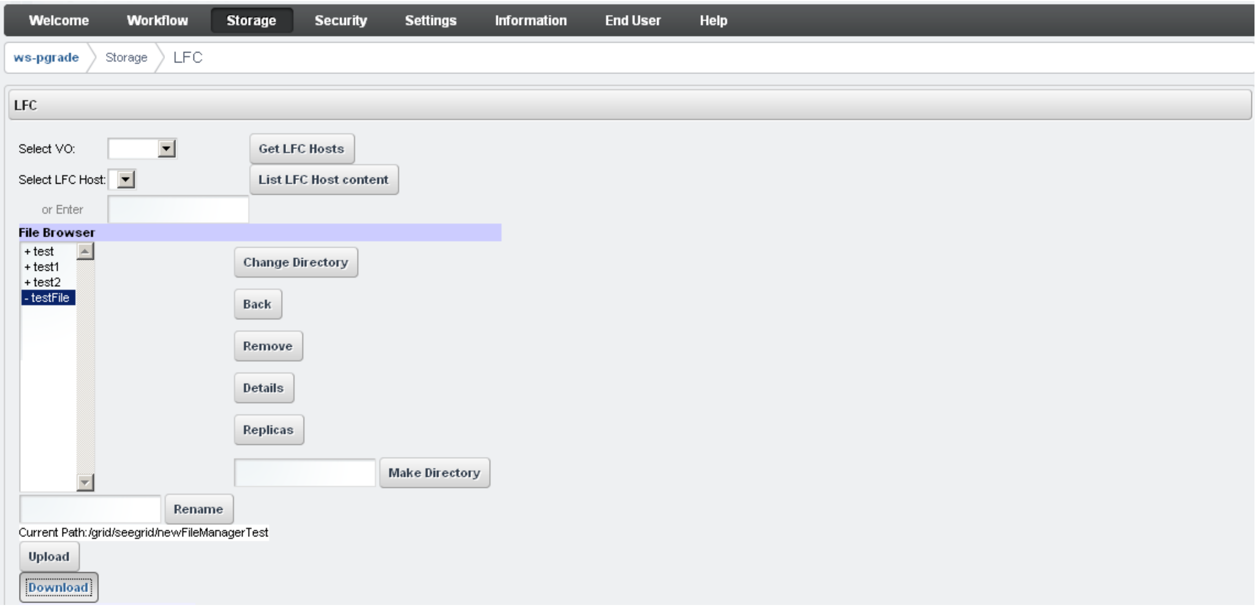
Current Path: /grid/seegrid/newFileManagerTest/test2

Message:

Appendix Figure 13.15 Uploaded file

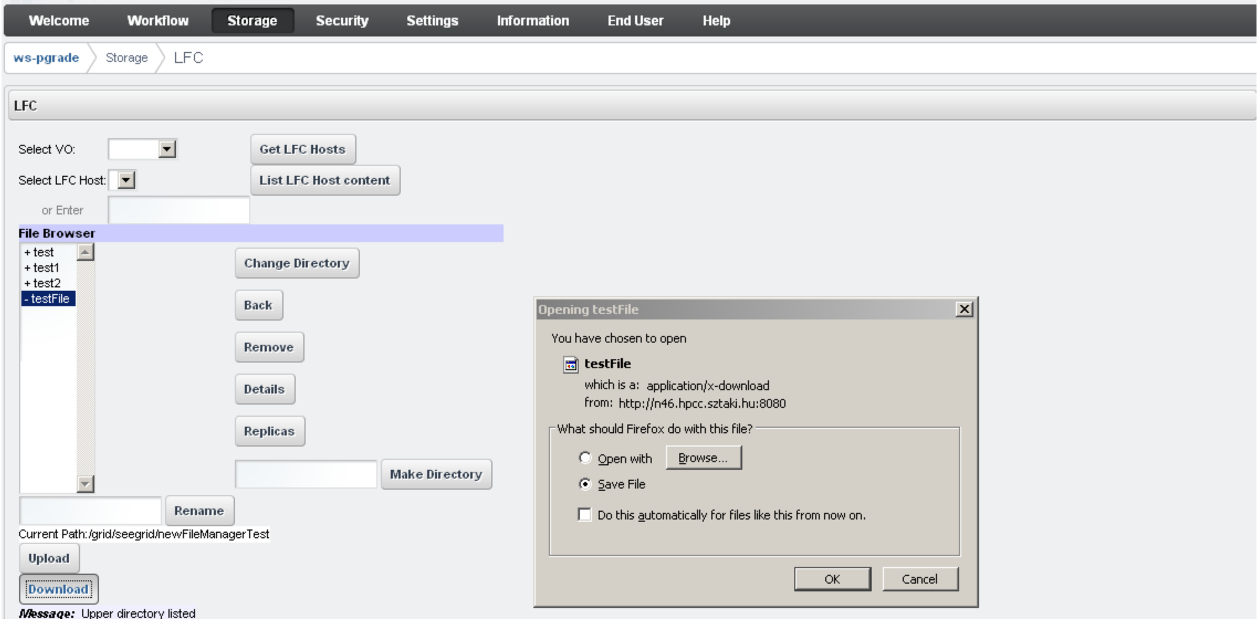
After selecting a file, the *Download* button on Figure 13.3 can be used to download that file. The file will be downloaded to the portal server and the user will be directed to the download page shown in Figure 15.17. The file will be removed from the portal server when user exits the download page.

For example, to download the file *testFile* under */grid/seegrid/newFileManagerTest* directory, contents of the directory */grid/seegrid/newFileManagerTest* should be listed. After selecting the file *testFile*, *Download* button should be clicked as shown in Figure 13.16. On the page shown in Figure 13.17, the file can be downloaded using the *Opening testFile* pop up window. The appearance of this pop up window indicates that the grid file has been downloaded from the grid infrastructure on to the WS-PGRADE infrastructure and can be downloaded from there on to the user machine by hitting *OK* button. In this case the destination of file can define by the browser dependent file download window shown in Figure 13.18.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
File Browser
+ test
+ test1
+ test2
- testFile
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download

Current Path:/grid/seegrid/newFileManagerTest

Appendix Figure 13.16 Select Grid file to download


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Get LFC Hosts
Select LFC Host:
List LFC Host content
or Enter
File Browser
+ test
+ test1
+ test2
- testFile
Change Directory
Back
Remove
Details
Replicas
Make Directory
Rename
Upload
Download
Opening testFile
Browse...
OK
Cancel

Current Path:/grid/seegrid/newFileManagerTest

Message: Upper directory listed

You have chosen to open

testFile

which is a: application/x-download

from: http://n46.hpcc.sztaki.hu:8080

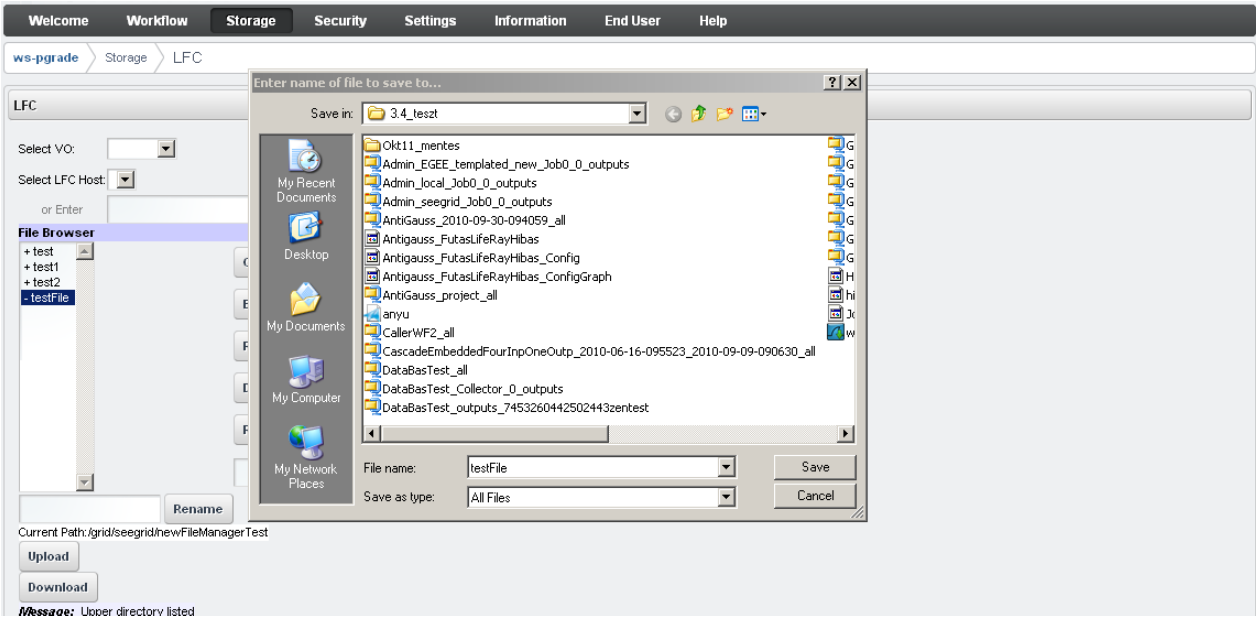
What should Firefox do with this file?

○ Open with

● Save File

☐ Do this automatically for files like this from now on.

Appendix Figure 13.17 The file is on the WS-PGRADE


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Select VO:
Select LFC Host:
or Enter
File Browser
Rename
Upload
Download
Enter name of file to save to...
Save in:
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
File name:
Save as type:
Save
Cancel

File Browser: + test, + test1, + test2, - testFile

Save in: 3.4_teszt

Okt11_mentes
Admin_EGEE_templated_new_Job0_0_outputs
Admin_local_Job0_0_outputs
Admin_seegrid_Job0_0_outputs
AntiGauss_2010-09-30-094059_all
Antigauss_FutasLifeRayHibas
Antigauss_FutasLifeRayHibas_Config
Antigauss_FutasLifeRayHibas_ConfigGraph
AntiGauss_project_all
anyu
CallerWF2_all
CascadeEmbeddedFourInpOneOutp_2010-06-16-095523_2010-09-09-090630_all
DataBasTest_all
DataBasTest_Collector_0_outputs
DataBasTest_outputs_7453260442502443zentest

File name: testFile

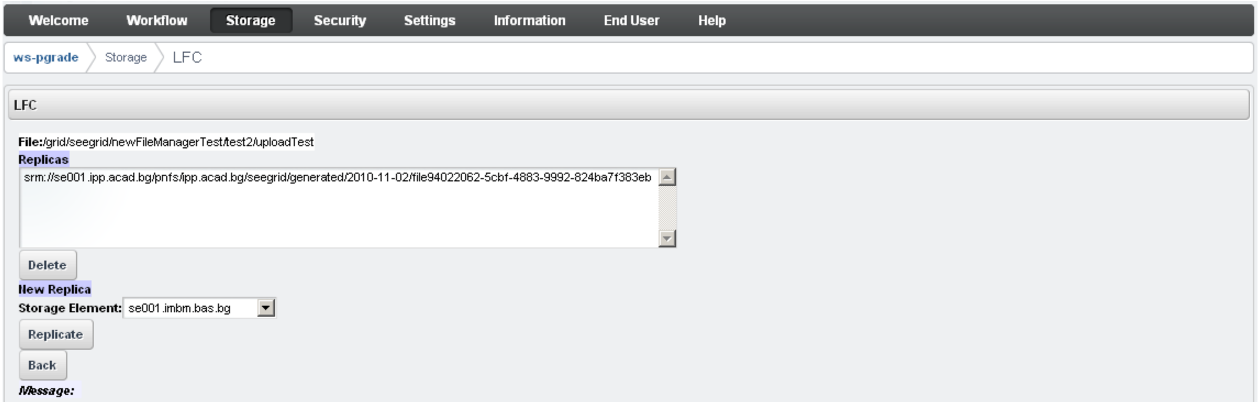
Save as type: All Files

Current Path:/grid/seegrid/newFileManagerTest

Message: Upper directory listed

Appendix Figure 13.18 Destination of downloaded file

After selecting a file and clicking on *Replicas* button on Figure 13.3, replicas of that file can be listed. On Figure 13.19, the single replica of the file */grid/seegrid/newFileManagerTest/test2/uploadTest* is displayed.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Delete
New Replica
Replicate
Back

File:/grid/seegrid/newFileManagerTest/test2/uploadTest

Replicas

srm://se001.ipp.acad.bg/pnfs/ipp.acad.bg/seegrid/generated/2010-11-02/file94022062-5cbf-4883-9992-824ba7f383eb

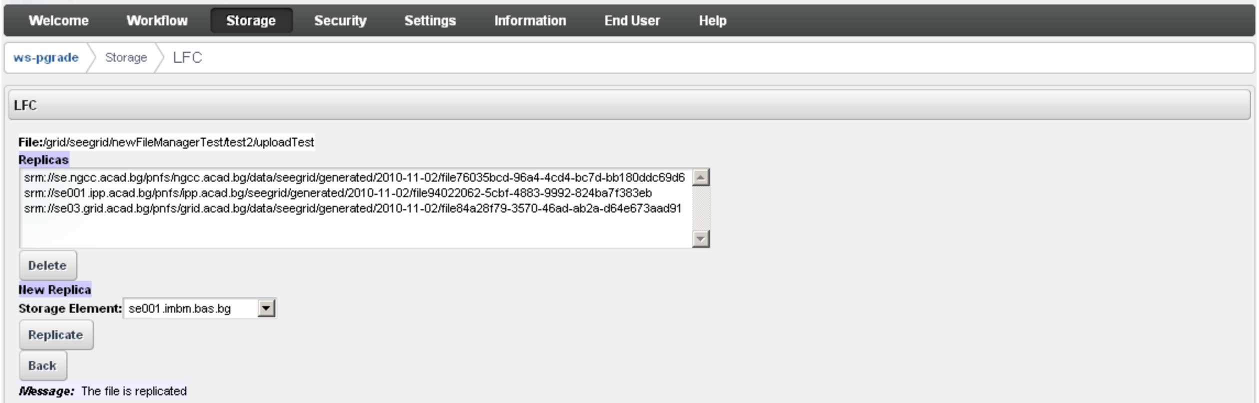
Storage Element: se001.imbm.bas.bg

Message:

Appendix Figure 13.19 List of replicas

To replicate a file should be listed replicas of file. On the page shown in Figure 13.19, a file can be replicated to the required storage element by selecting a storage element and clicking on *Replicate* button.

On Figure 13.20, the file */grid/seegrid/newFileManagerTest/test2/uploadTest* is replicated to the storage elements *se.ngcc.acad.bg* and *se03.grid.acad.bg*.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Delete
Replicate
Back

File:/grid/seegrid/newFileManagerTest/test2/uploadTest

Replicas

srm://se.ngcc.acad.bg/pnfs/ngcc.acad.bg/data/seegrid/generated/2010-11-02/file76035bcd-96a4-4cd4-bc7d-bb180ddc69d6
srm://se001.ipp.acad.bg/pnfs/ipp.acad.bg/seegrid/generated/2010-11-02/file94022062-5cbf-4883-9992-824ba7f383eb
srm://se03.grid.acad.bg/pnfs/grid.acad.bg/data/seegrid/generated/2010-11-02/file84a28f79-3570-46ad-ab2a-d64e673aad91

New Replica

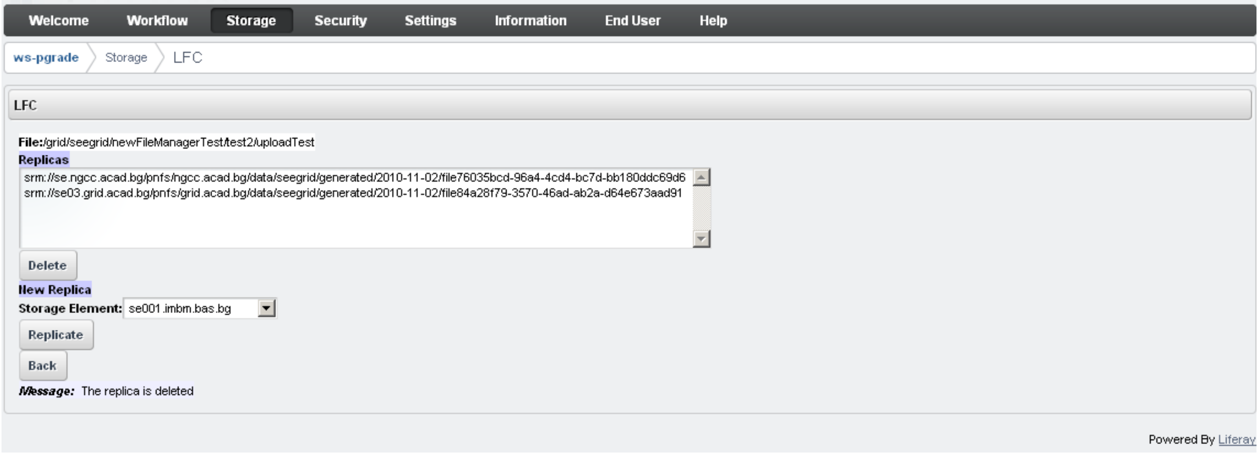
Storage Element: se001.imbm.bas.bg

Message: The file is replicated

Appendix Figure 13.20 List of replicas after replicating

To delete a replica of a file, replicas of the file should be listed. On the page shown in Figure 13.20, a replica of a file can be deleted by selecting the required replica and clicking the *Delete* button.

On Figure 13.21, replica of the file */grid/seegrid/newFileManagerTest/test2/uploadTest* on the storage element *se001.ipp.acad.*bg is deleted.


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Storage
LFC
LFC
Delete
Replicate
Back
Powered By Liferay

File:/grid/seegrid/newFileManagerTest/test2/uploadTest

Replicas

srm://se.ngcc.acad.bg/pnfs/ngcc.acad.bg/data/seegrid/generated/2010-11-02/file76035bcd-96a4-4cd4-bc7d-bb180ddc69d6
srm://se03.grid.acad.bg/pnfs/grid.acad.bg/data/seegrid/generated/2010-11-02/file84a28f79-3570-46ad-ab2a-d64e673aad91

New Replica

Storage Element: se001.imbm.bas.bg

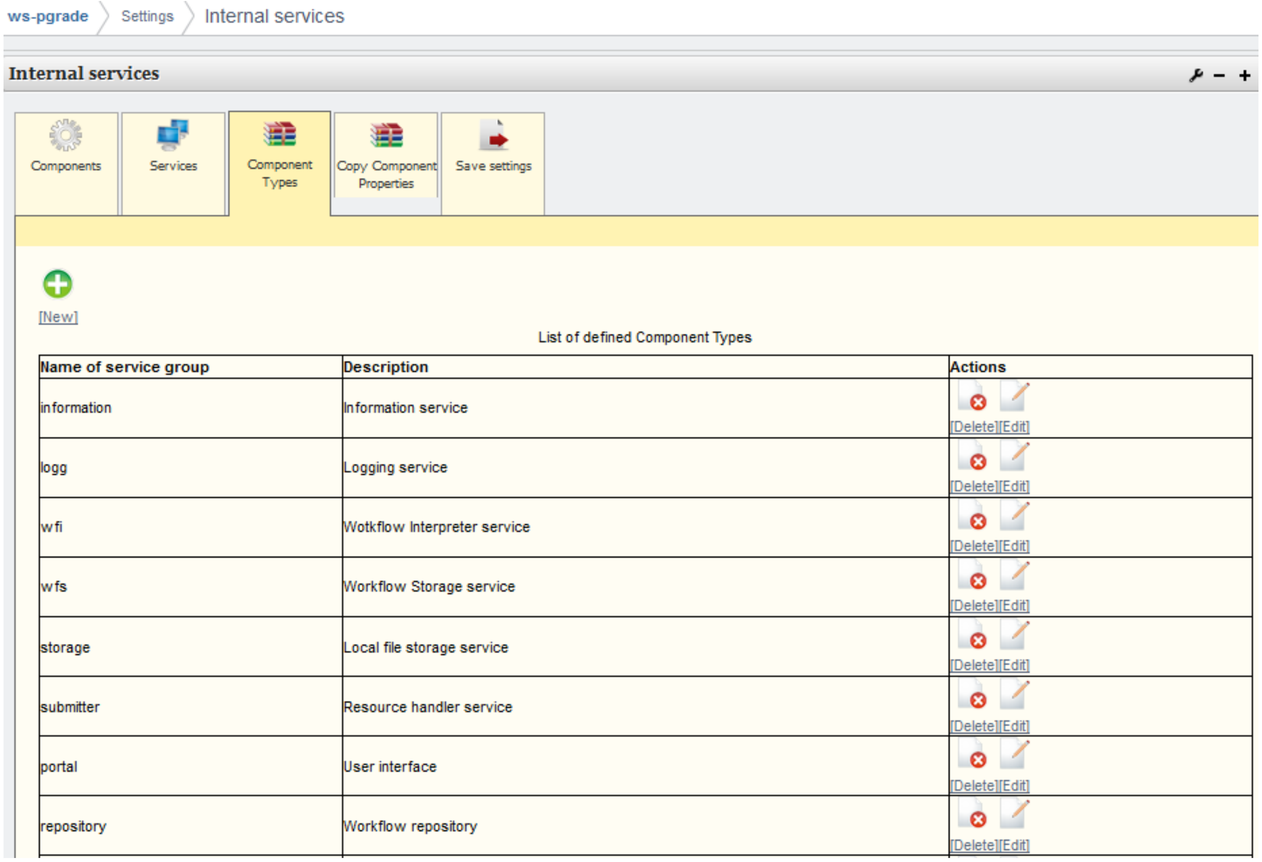
Message: The replica is deleted

Appendix Figure 13.21 List of remaining replicas

14. Internal Services Group

14.1 Component Types

Notes: Edit modifies only the *Description* the functionality. It has no semantic significance. This list of *Component Types* enumerates all *Component Types* needed in gUSE. However, it is possible to define a new *Component Type* by clicking the *New* button.

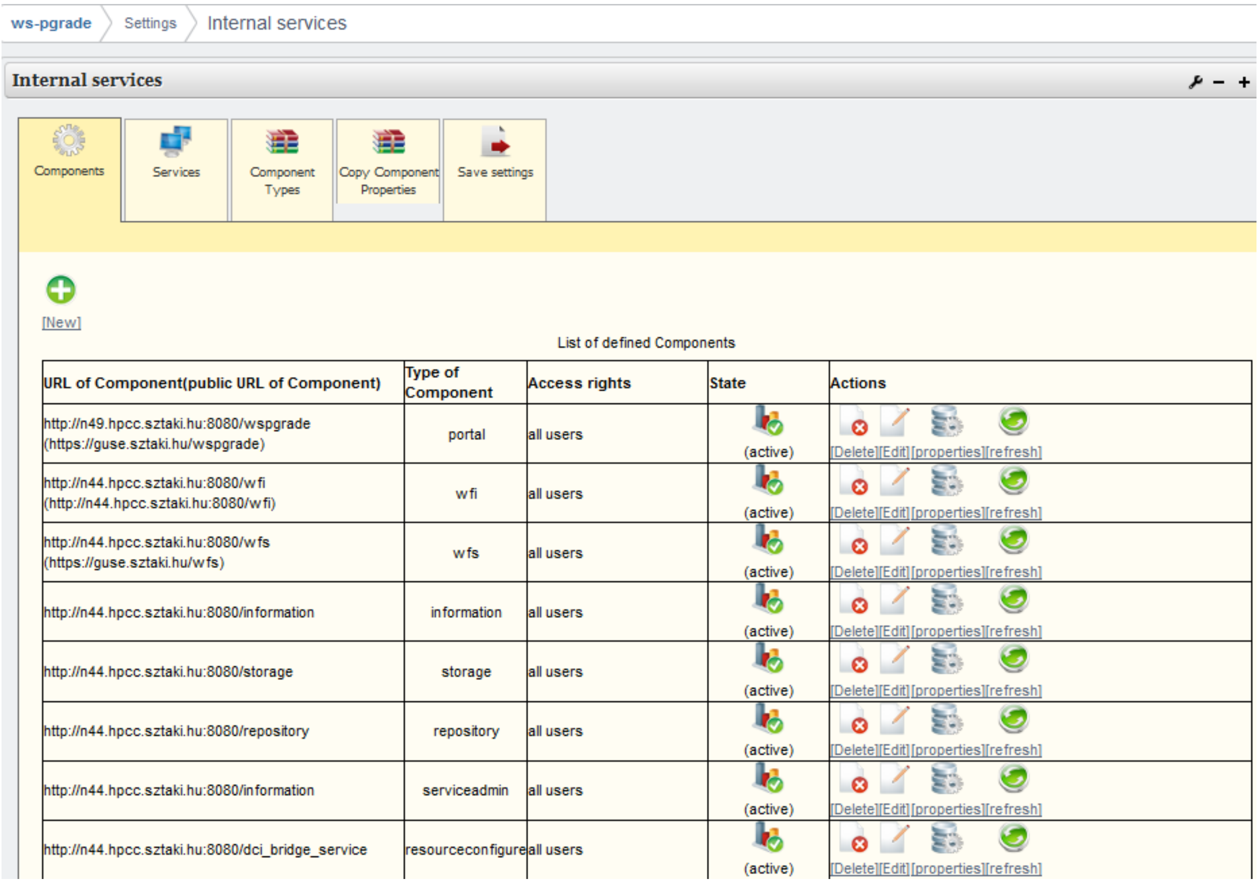

ws-pgrade
Settings
Internal services
Internal services
Components
Services
Component Types
Copy Component Properties
Save settings
[New]

List of defined Component Types

Name of service group	Description	Actions
information	Information service	[Delete][Edit]
logg	Logging service	[Delete][Edit]
wfi	Wotkflow Interpreter service	[Delete][Edit]
wfs	Workflow Storage service	[Delete][Edit]
storage	Local file storage service	[Delete][Edit]
submitter	Resource handler service	[Delete][Edit]
portal	User interface	[Delete][Edit]
repository	Workflow repository	[Delete][Edit]

Appendix Figure 14.1 List of Component types

14.2 Components



List of defined Components

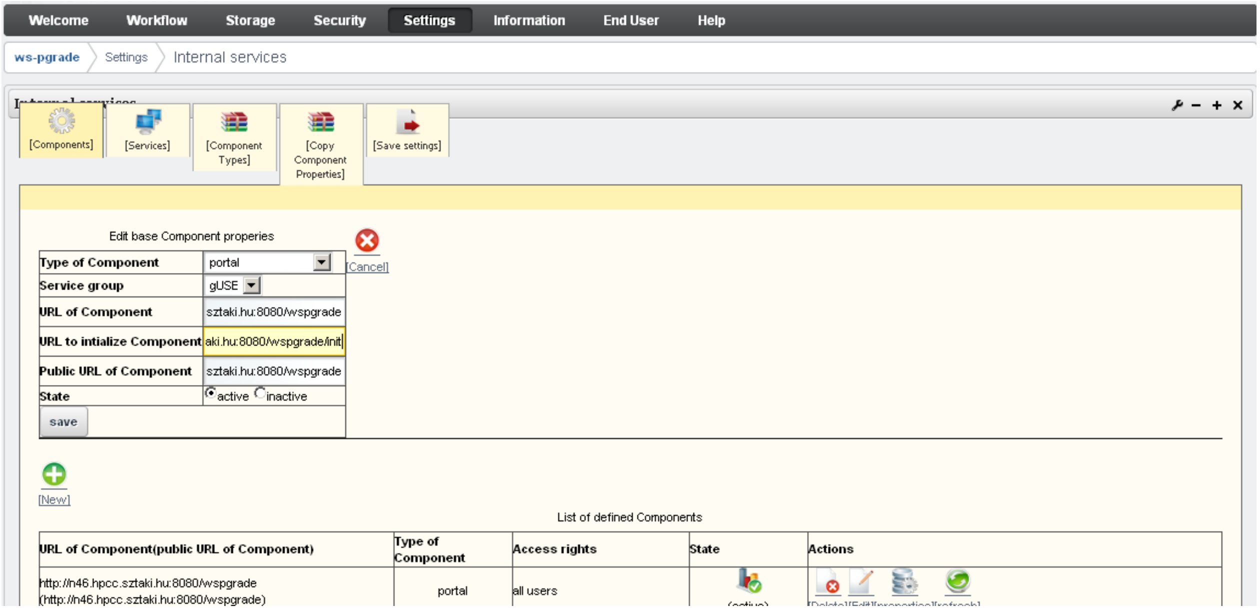
URL of Component(public URL of Component)	Type of Component	Access rights	State	Actions
http://n49.hpcc.sztaki.hu:8080/wspgrade (https://guse.sztaki.hu/wspgrade)	portal	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/wfi (http://n44.hpcc.sztaki.hu:8080/wfi)	wfi	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/wfs (https://guse.sztaki.hu/wfs)	wfs	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/information	information	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/storage	storage	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/repository	repository	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/information	serviceadmin	all users	(active)	[Delete][Edit][properties][refresh]
http://n44.hpcc.sztaki.hu:8080/dci_bridge_service	resourceconfigure	all users	(active)	[Delete][Edit][properties][refresh]

Appendix Figure 14.2 List of existing Components

The common (generic) parameters of a component can be changed by clicking the *Edit* button (see 14.2.1). The *Component Type* dependent parameters can be maintained by clicking *Refresh* button (see 14.2.2).

When a new component will be created (by clicking the *New* button) only the common parameters must be defined. The properties of an existing component can be copied with a separate menu in a single step. (See 14.4.) The component can be initialized by clicking the refresh button. All referenced services will be initialized.

14.2.1 Component Generic Part


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Settings
Internal services
[Components]
[Services]
[Component Types]
[Copy Component Properties]
[Save settings]
[Cancel]
save
[New]

Edit base Component properies

Type of Component	portal
Service group	gUSE
URL of Component	sztaki.hu:8080/wspgrade
URL to intialize Component	aki.hu:8080/wspgrade/init
Public URL of Component	sztaki.hu:8080/wspgrade
State	● active ○ inactive

List of defined Components

URL of Component(public URL of Component)	Type of Component	Access rights	State	Actions
http://n46.hpcc.sztaki.hu:8080/wspgrade (http://n46.hpcc.sztaki.hu:8080/wspgrade)	portal	all users		

Appendix Figure 14.3 Component Generic Part accessible by "Edit"

Notes:

-A *Component* refers to a real computational resource of a service - therefore the definition of the URL(s) needed.

-It must reference an existing *Service Group*.

-It must have a predefined *Component Type*.

- A component can be activated/deactivated in runtime.

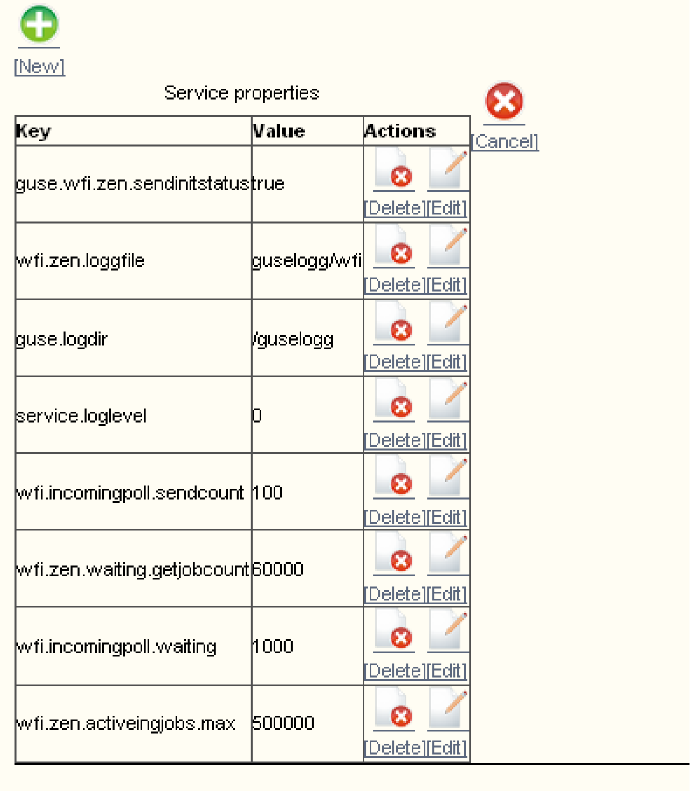
14.2.2 Component - Type dependent part

Component Type dependent part - here CT="wfi"

Notes:

Values of existing properties can be changed by clicking the *Edit* button.

New properties (key value pairs) can be created by clicking the *New* button.

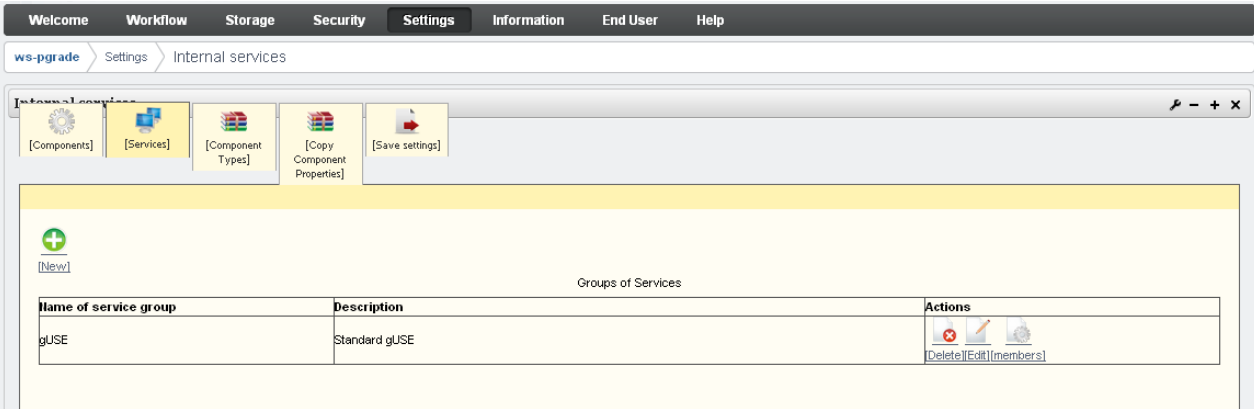


Service properties

Key	Value	Actions
guse.wfi.zen.sendinitstatus	true	[Delete][Edit]
wfi.zen.loggfile	guselogg/wfi	[Delete][Edit]
guse.logdir	/guselogg	[Delete][Edit]
service.loglevel	0	[Delete][Edit]
wfi.incomingpoll.sendcount	100	[Delete][Edit]
wfi.zen.waiting.getjobcount	60000	[Delete][Edit]
wfi.incomingpoll.waiting	1000	[Delete][Edit]
wfi.zen.activeingjobs.max	500000	[Delete][Edit]

Appendix Figure 14.4 Component Type dependent part - here

14.3 Services


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Settings
Internal services
[Components]
[Services]
[Component Types]
[Copy Component Properties]
[Save settings]
[New]

Groups of Services

Name of service group	Description	Actions
gUSE	Standard gUSE	[Delete][Edit][members]

Appendix Figure 14.5 Defined Service Groups

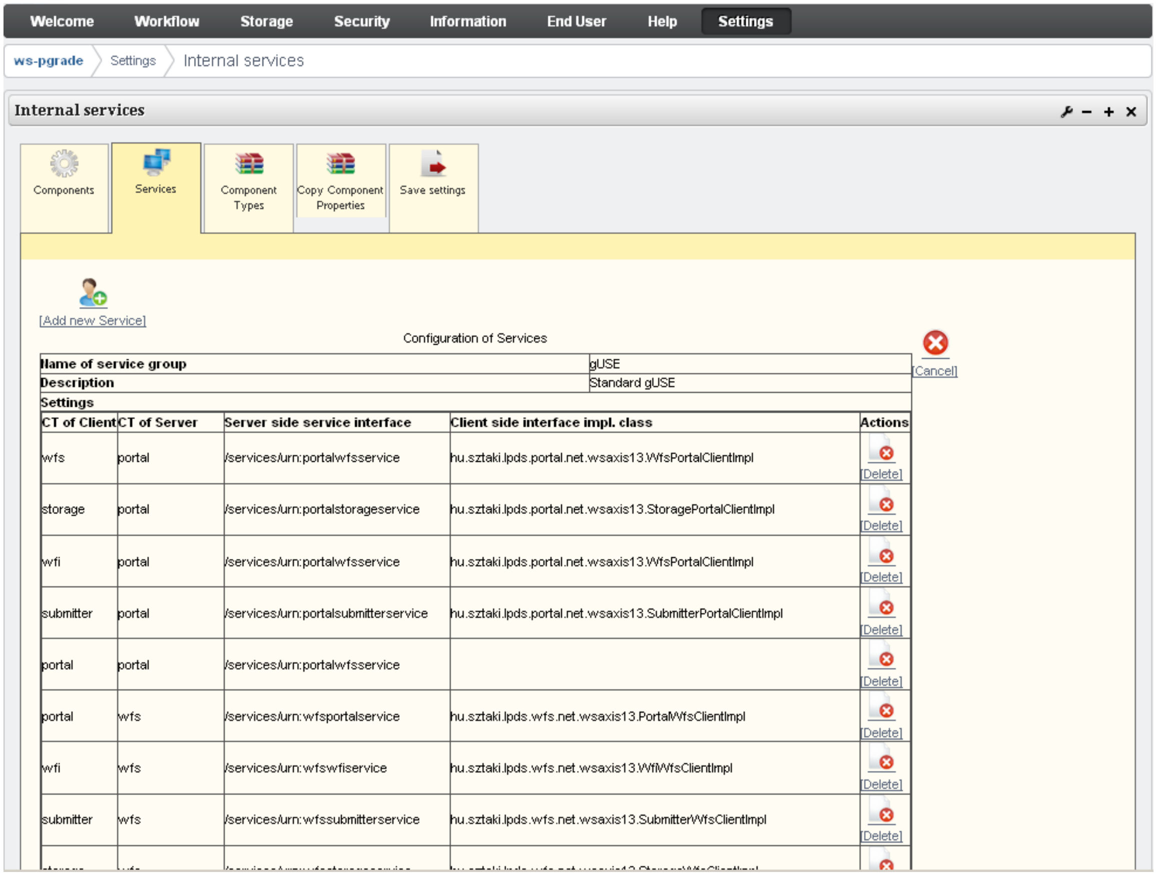
Notes:

At present the single Service Group is the "*gUSE*" .

A new group can be created by clicking the *New* button.

Edit modifies only the "*Description*" the functionality. It has no semantic significance.

Clicking on Members the defined Services can be maintained (see 14.3.1)


Welcome
Workflow
Storage
Security
Information
End User
Help
Settings
ws-pgrade
Settings
Internal services
Internal services
Components
Services
Component Types
Copy Component Properties
Save settings
[Add new Service]
[Cancel]

Configuration of Services

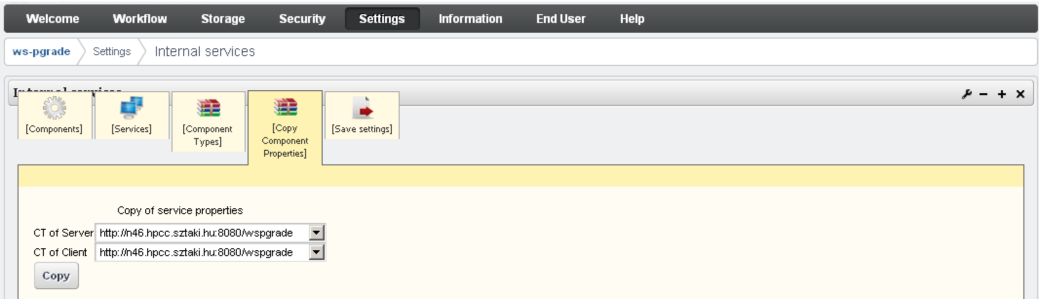
Name of service group	gUSE
Description	Standard gUSE
Settings	

CT of Client	**CT of Server**	**Server side service interface**	**Client side interface impl. class**	**Actions**
wfs	portal	/services/urn:portalwfsservice	hu.sztaki.lpds.portal.net.wsaxis13.WfsPortalClientImpl	[Delete]
storage	portal	/services/urn:portalstorageservice	hu.sztaki.lpds.portal.net.wsaxis13.StoragePortalClientImpl	[Delete]
wfi	portal	/services/urn:portalwfsservice	hu.sztaki.lpds.portal.net.wsaxis13.WfsPortalClientImpl	[Delete]
submitter	portal	/services/urn:portalsubmitterservice	hu.sztaki.lpds.portal.net.wsaxis13.SubmitterPortalClientImpl	[Delete]
portal	portal	/services/urn:portalwfsservice		[Delete]
portal	wfs	/services/urn:wfsportalservice	hu.sztaki.lpds.wfs.net.wsaxis13.PortalWfsClientImpl	[Delete]
wfi	wfs	/services/urn:wfswfiservice	hu.sztaki.lpds.wfs.net.wsaxis13.WfiWfsClientImpl	[Delete]
submitter	wfs	/services/urn:wfssubmitterservice	hu.sztaki.lpds.wfs.net.wsaxis13.SubmitterWfsClientImpl	[Delete]

Appendix Figure 14.6 List of existing Service call possibilities among the Components

A new Service can be defined by clicking the *Add new Service* button.

14.4 Copy Component Properties


Welcome
Workflow
Storage
Security
Settings
Information
End User
Help
ws-pgrade
Settings
Internal services
[Components]
[Services]
[Component Types]
[Copy Component Properties]
[Save settings]
Copy

Copy of service properties

CT of Server http://n46.hpcc.sztaki.hu:8080/wspgrade
CT of Client http://n46.hpcc.sztaki.hu:8080/wspgrade

Appendix Figure 14.7

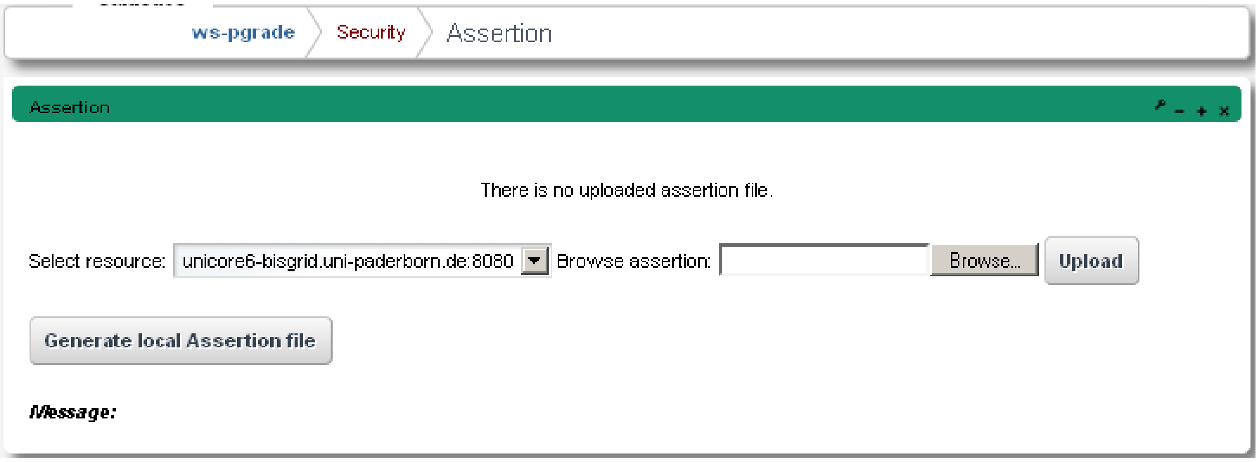
15. The Assertion Menu

The *Assertion* menu supports the security concept of the UNICORE middleware.

Replacing the MyProxy Server used by most Globus like grids the assertion concept supports the local generation of short term proxy certificates avoiding the potentially dangerous transfer of the secure key file on to the remote MyProxy Server.

The assertion replaces the properties of the proxy certificate. The assertion file will be generated, on the local machine of the user. The portlet controls the life cycle of the assertion file.

A new assertion file can be generated on the entry page of the portlet:



There is no uploaded assertion file.

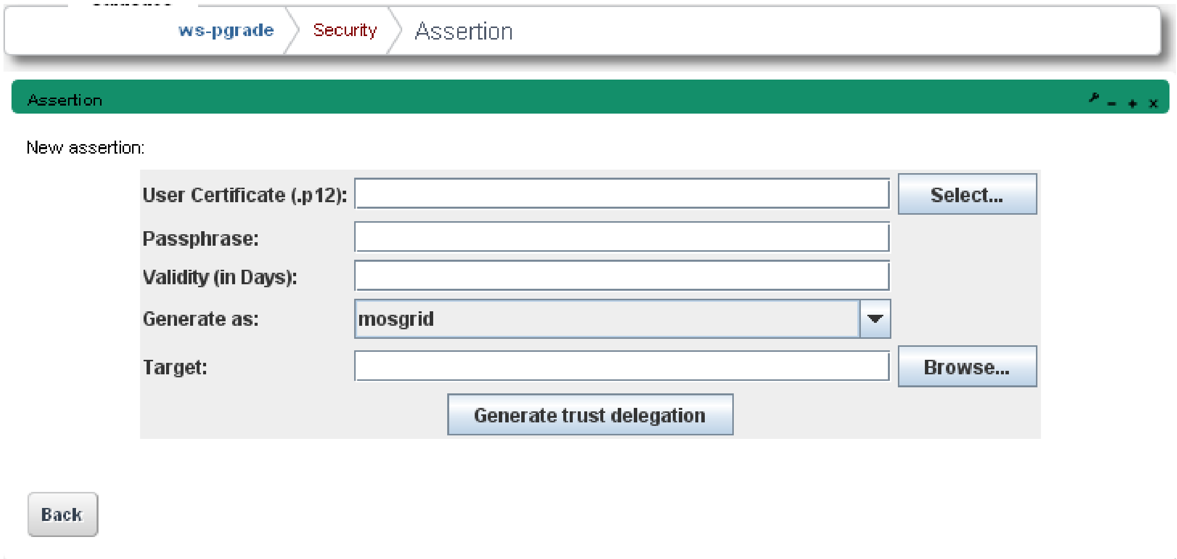
Select resource: unicore6-bisgrid.uni-paderborn.de:8080

Message:

ws-pgrade
Security
Assertion
Assertion
Browse assertion:
Browse...
Upload
Generate local Assertion file

Appendix Figure 15.1 The Assertion menu - initial view

An applet will be embedded in the portlet by clicking the Generate local Assertion file button:



New assertion:

Generate as: mosgrid

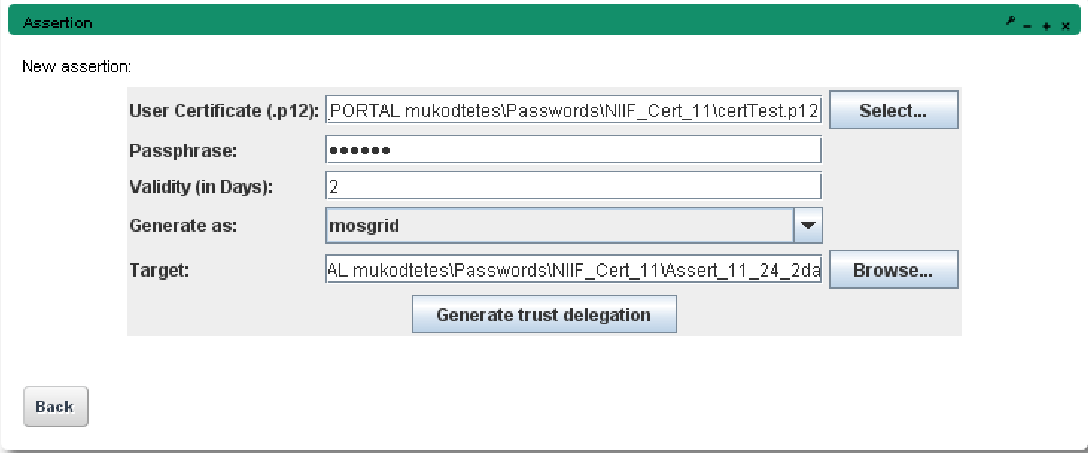
ws-pgrade
Security
Assertion
Assertion
User Certificate (.p12):
Select...
Passphrase:
Validity (in Days):
Target:
Browse...
Generate trust delegation
Back

Appendix Figure 15.2 The Assertion menu - initial view of downloaded applet

Notes:

- *User certificate*: Here the *PKCS12* format of the long term user certificate is expected for the proxy generation. The path of the proper file must be defined by the *Select…* file browser.
- *Passphrase*: The passphrase is the password belonging to the secure key part of the long term user certificate.
- *Validity* (in Days): The user must define the lifetime of the assertion file to be generated.
- *Generate as*: The user must select one among the available groups of the UNICORE resources where the assertion will be is accepted i.e. the DN part of the long term user certificate is known and welcomed.
- *Target*: Place of the *Assert* file to be generated. The file browser Browse helps the selection:

An example:

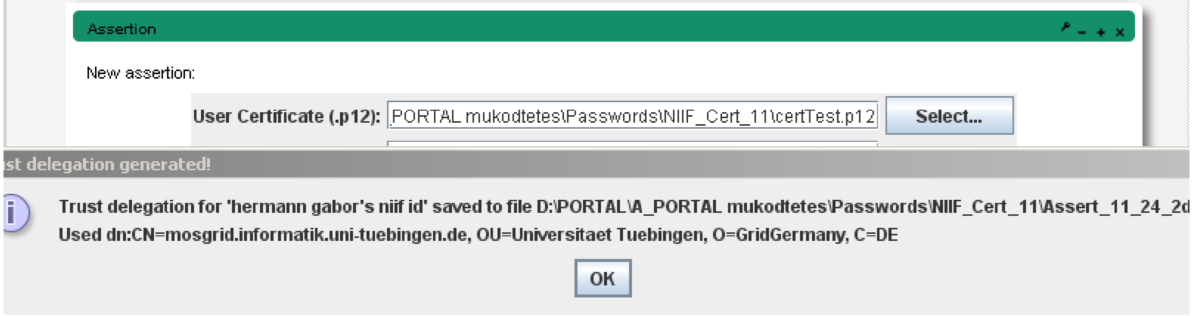


User Certificate (.p12): PORTAL mukodtetes\Passwords\NIIF_Cert_11\certTest.p12
Passphrase: ••••••
Validity (in Days): 2
Generate as: mosgrid
Target: AL mukodtetes\Passwords\NIIF_Cert_11\Assert_11_24_2da

Appendix Figure 15.3 Defined assertion to be saved locally

The generation can be confirmed by clicking the button Generate trust delegation.

The system reports the success:



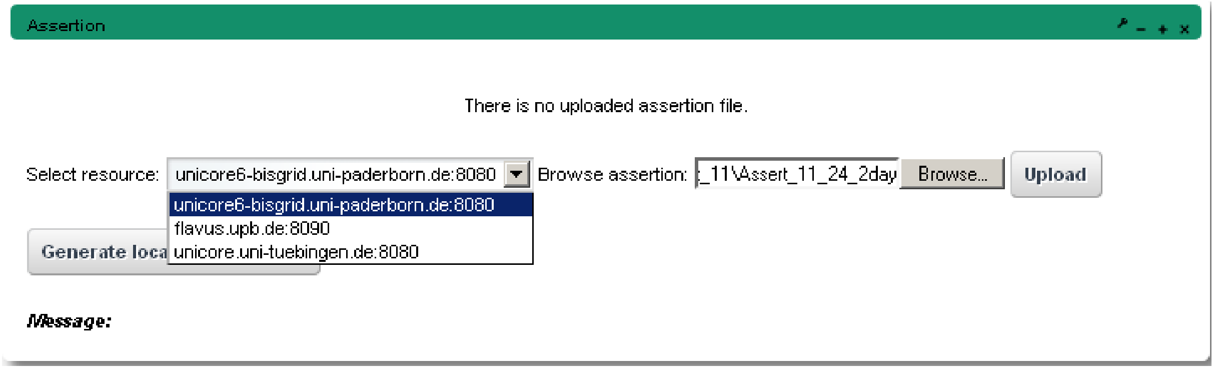
User Certificate (.p12): PORTAL mukodtetes\Passwords\NIIF_Cert_11\certTest.p12

st delegation generated!

Trust delegation for 'hermann gabor's niif id' saved to file D:\PORTAL\A_PORTAL mukodtetes\Passwords\NIIF_Cert_11\Assert_11_24_2d
Used dn:CN=mosgrid.informatik.uni-tuebingen.de, OU=Universitaet Tuebingen, O=GridGermany, C=DE

Appendix Figure 15.4 Generation report

Acknowledging this message by clicking *OK* and releasing the applet by the Back button the menu returns to the start page where the user is prompted to upload the *Assertion* file:


Assertion
Browse...
Upload
Generate loca
unicore6-bisgrid.uni-paderborn.de:8080
flavus.upb.de:8090
unicore.uni-tuebingen.de:8080

There is no uploaded assertion file.

Select resource: unicore6-bisgrid.uni-paderborn.de:8080

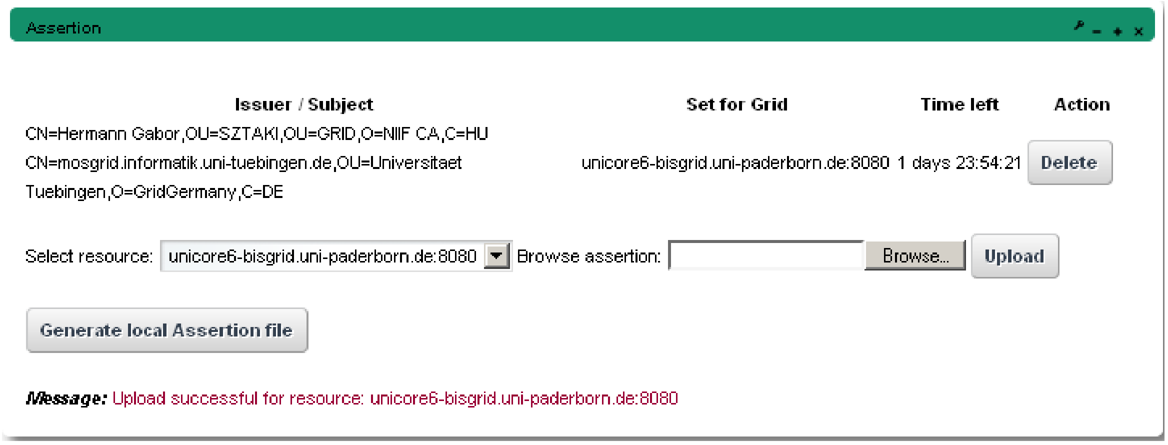
Browse assertion: _11\Assert_11_24_2day

Message:

Appendix Figure 15.5 Assertion upload page

Notes:

- Select resource: The resource must be selected where the user wants to submit jobs by the help of the assertion file to be uploaded.
- Browse assertion: The local storage place of the existing assertion file must be defined by the help of the file browser *Browse*. (See the field Target of Appendix Figure 16.3).
- Clicking the *Upload* button confirms the operation and the recently uploaded assertion appears on the portal server:


Assertion
Delete
Browse...
Upload
Generate local Assertion file

Issuer / Subject	Set for Grid	Time left	Action
CN=Hermann Gabor,OU=SZTAKI,OU=GRID,O=NIIF CA,C=HU CN=mosgrid.informatik.uni-tuebingen.de,OU=Universitaet Tuebingen,O=GridGermany,C=DE	unicore6-bisgrid.uni-paderborn.de:8080	1 days 23:54:21	Delete

Select resource: unicore6-bisgrid.uni-paderborn.de:8080

Browse assertion:

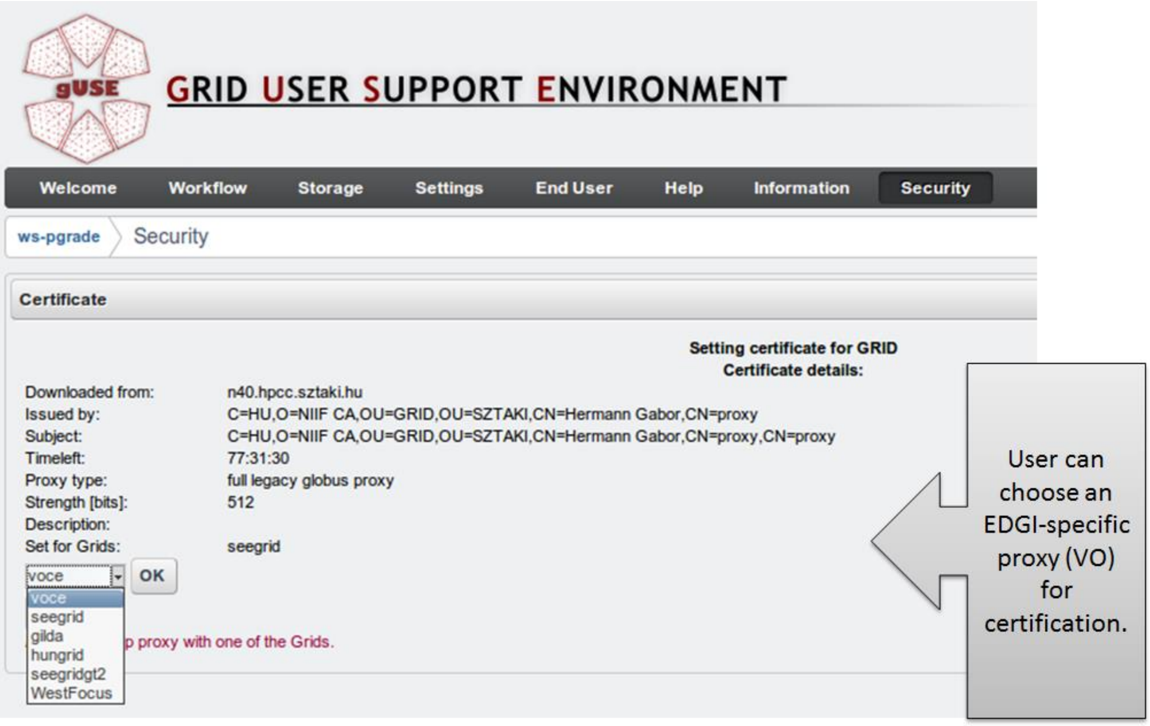
Message: Upload successful for resource: unicore6-bisgrid.uni-paderborn.de:8080

Appendix Figure 15.6 Usable uploaded assertion

16. The EDGI-based Functions

EDGI integrates software components of some middleware into Service Grid - Desktop Grid platforms for service provision and as a result EDGI will extend ARC, gLite and UNICORE grids with volunteer and institutional DG systems. By EDGI-specific middleware support it is possible to use the WS-PGRADE -> Service Grid -> Desktop Grid (currently gLite-based EDGI VO) path in order to run applications (from EDGI Application Repository) on the EDGI (SG -> DG) infrastructure. From WS-PGRADE users can run workflows whose jobs can be configured to EDGI.

In practice, the user's executable program for job configuration and submission is always in the EDGI Application Repository (AR), not in a local place. The first step on EDGI function in the EDGI-specific workflow settings is the certificate settings (Figure Appendix 16.1).


gUSE
GRID USER SUPPORT ENVIRONMENT
Welcome
Workflow
Storage
Settings
End User
Help
Information
Security
ws-pgrade
Security
Certificate
voce
OK
voce
seegrid
gilda
hungrid
seegridgt2
WestFocus

Setting certificate for GRID
Certificate details:

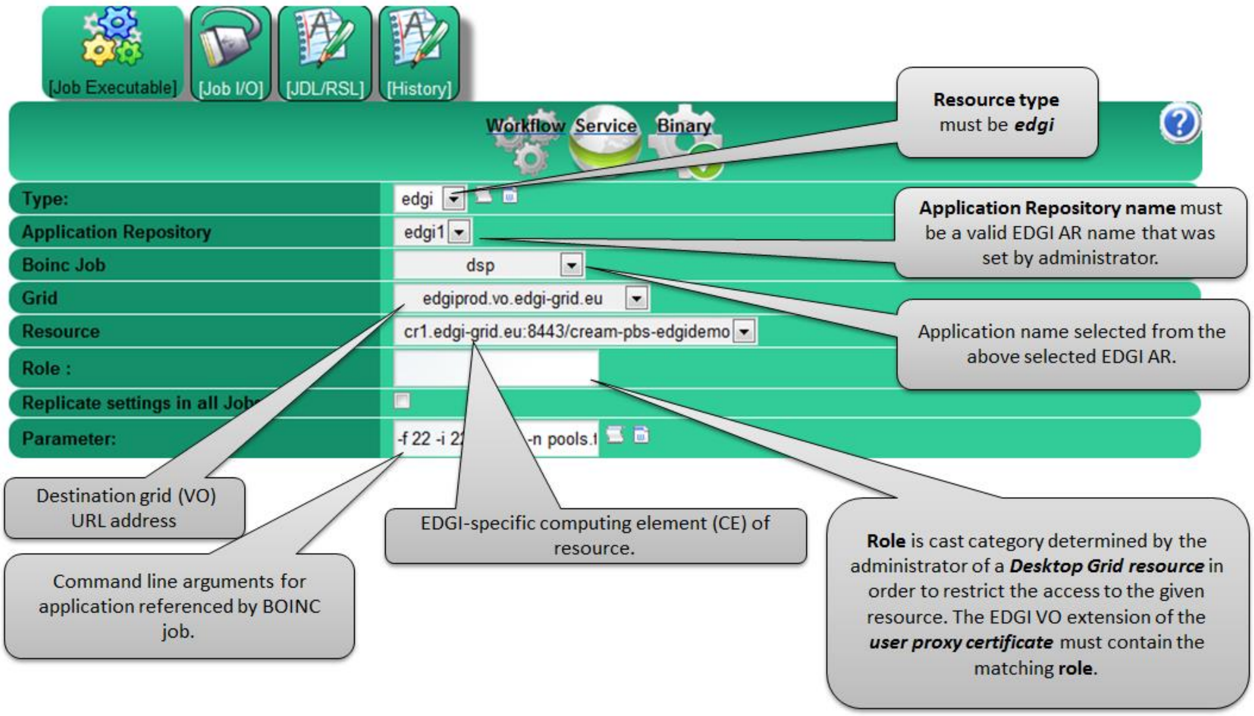
Downloaded from: n40.hpcc.sztaki.hu
Issued by: C=HU,O=NIIF CA,OU=GRID,OU=SZTAKI,CN=Hermann Gabor,CN=proxy
Subject: C=HU,O=NIIF CA,OU=GRID,OU=SZTAKI,CN=Hermann Gabor,CN=proxy,CN=proxy
Timeleft: 77:31:30
Proxy type: full legacy globus proxy
Strength [bits]: 512
Description:
Set for Grids: seegrid

p proxy with one of the Grids.

User can choose an EDGI-specific proxy (VO) for certification.

Appendix Figure 16.1 EDGI-specific proxy setting

The essential EDGI-specific settings in *Job Executable* tab summarized by Figure 16.2.



Type: edgi
Application Repository: edgi1
Boinc Job: dsp
Grid: edgiprod.vo.edgi-grid.eu
Resource: cr1.edgi-grid.eu:8443/cream-pbs-edgidemo
Role :
Replicate settings in all Jobs: ☐
Parameter: -f 22 -i 2 -n pools.t

Resource type must be ***edgi***

Application Repository name must be a valid EDGI AR name that was set by administrator.

Application name selected from the above selected EDGI AR.

Destination grid (VO) URL address

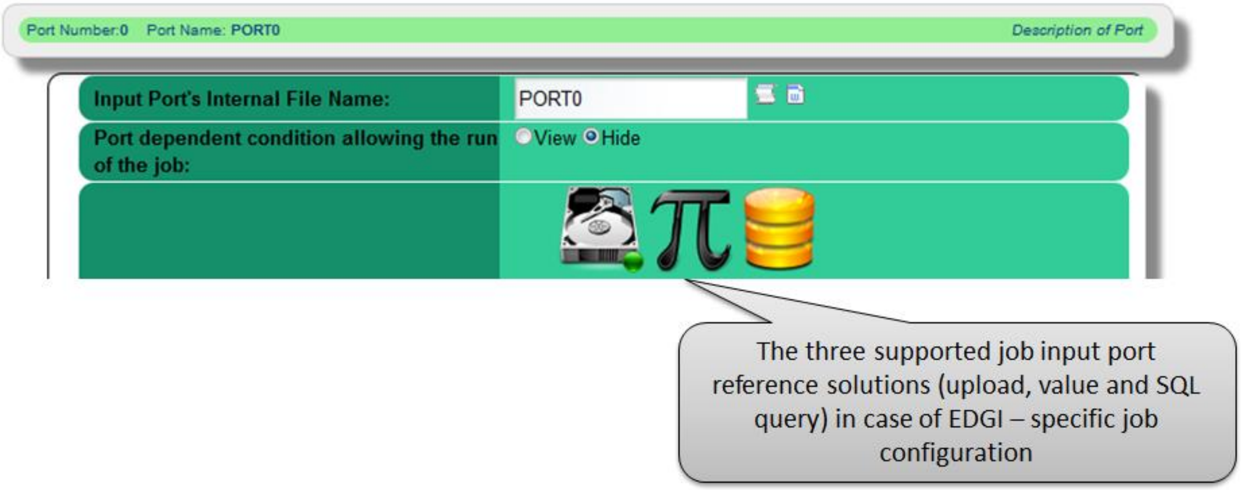
Command line arguments for application referenced by BOINC job.

EDGI-specific computing element (CE) of resource.

Role is cast category determined by the administrator of a ***Desktop Grid resource*** in order to restrict the access to the given resource. The EDGI VO extension of the ***user proxy certificate*** must contain the matching **role**.

Appendix Figure 16.2 EDGI-specific settings in Job Executable tab

In case of EDGI job configuration the Remote File reference is not supported in the Job I/O tab (Appendix Figure 16.3)



Port Number:0 Port Name: PORT0

Input Port's Internal File Name: PORT0

Port dependent condition allowing the run of the job: ○ View ● Hide

The three supported job input port reference solutions (upload, value and SQL query) in case of EDGI – specific job configuration

Appendix Figure 16.3 The three possible input port reference solution at EDGI-based job configuration

17. Job Submission to Cloud by the CloudBroker Platform

The CloudBroker (CB) platform is an application store for high performance computing in the cloud. Through the CloudBroker menu of WS-PGRADE/gUSE different scientific and technical applications can be accessed, selected and immediately executed in the cloud, pay-per-use. Softwares (in cloud terminology: SaaS - Software as a Service) registered in the CB platform are stored in a repository, which can be queried by gUSE.

Thus, the user can run applications from CB repository as workflow nodes.

17.1 Registration

In order to be able access the CB platform you have to own username and password provided by CloudBroker GmbH after registration – which is used in every communication with the platform. Note: the WS-PGRADE portal account is not enough to submit jobs.

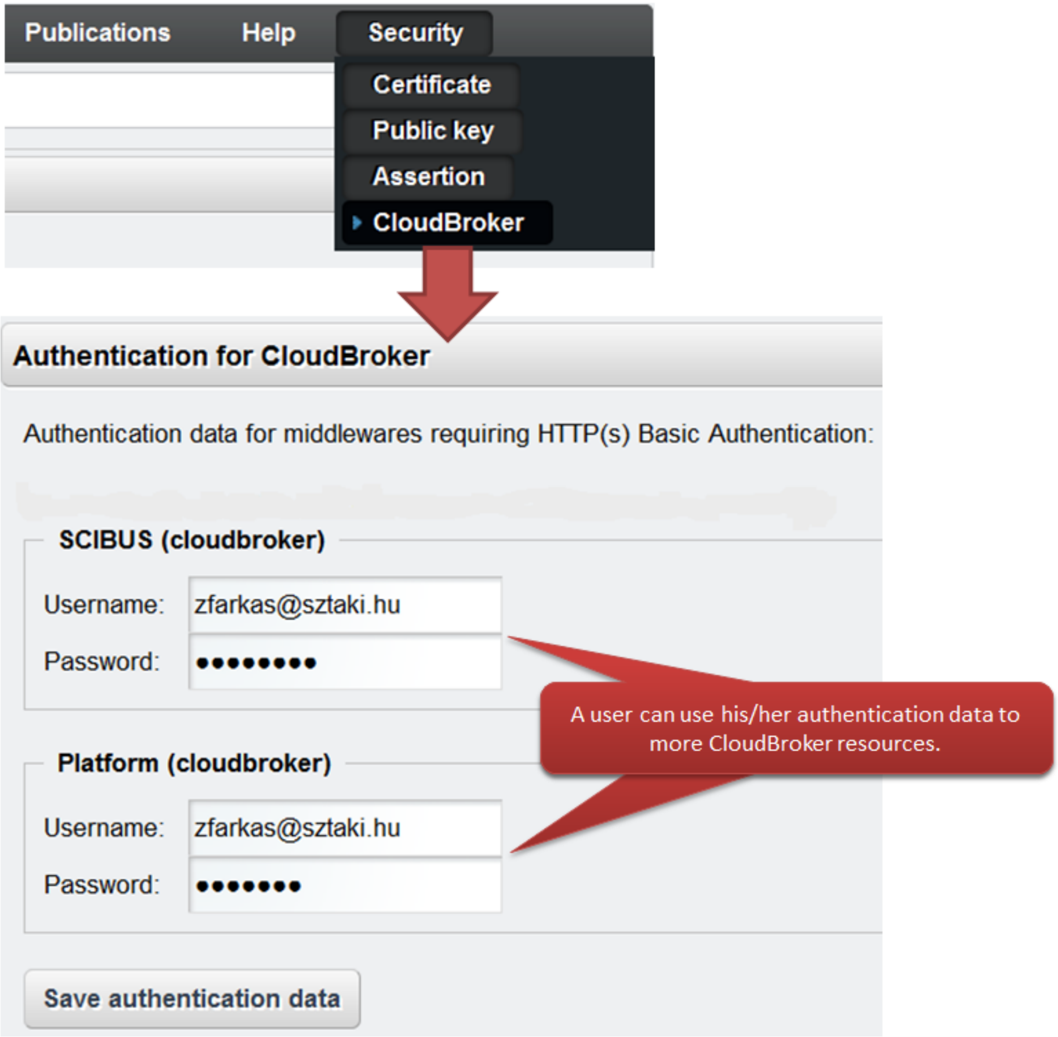
Basically, there are two types of users in CB environment: administrators and standard users. Administrators typically represent organizations and have the potential to create new users (manage or delete) belonging to the same organization, whereas standard users (as well as administrators) can query repository and execute softwares (made public). Administrators can deploy new software that is in "private" status initially. Private status means only administrators can see them at listing the repository and only administrators can run, respectively. Once the software has been tested, i.e. they can really be run on the deployed resource and works as expected, it may be published for use by the organization or by anyone accessing the CB platform by setting software status to "public".

There are two options to get CB platform account:

1. The administrator registers a new organization together with her/his new personal account in this page: https://platform.cloudbroker.com/registration/new_user_organization. After the registration process, the administrator need to define and deploy resources and softwares that will be used in the registered new organization. *To more details about administrative operations, please see chapter V in the Admin Manual.*
2. The standard user will be registered to an already existed organization by the organization administrator (the user asks a registration of her/his organization administrator) and she/he got an account from the administrator. The user can only use the resources and softwares which are used by her/his organization.

Once the registration process is finished, the user can give in WS-PGRADE the necessary username and password data used to query available software on the CB platform at job configuration or submitting jobs at workflow executions, respectively, by selecting Security/CloudBroker menu. It is shown in Figure 17.1. As a result of clicking on *Save authentication data* button, username and password information will be saved. If you clear Username (and/or Password) field(s), containing authentication file will be deleted from the file system (not only its content).

Note again: the authentication information associated with the particular user only logged-in to the portal; the given username and password are not shared among other users (though they can set the same information if they know and allowed to use).



Authentication for CloudBroker

Authentication data for middlewares requiring HTTP(s) Basic Authentication:

SCIBUS (cloudbroker)

Username: zfarkas@sztaki.hu
Password: ••••••••

Platform (cloudbroker)

Username: zfarkas@sztaki.hu
Password: •••••••

A user can use his/her authentication data to more CloudBroker resources.

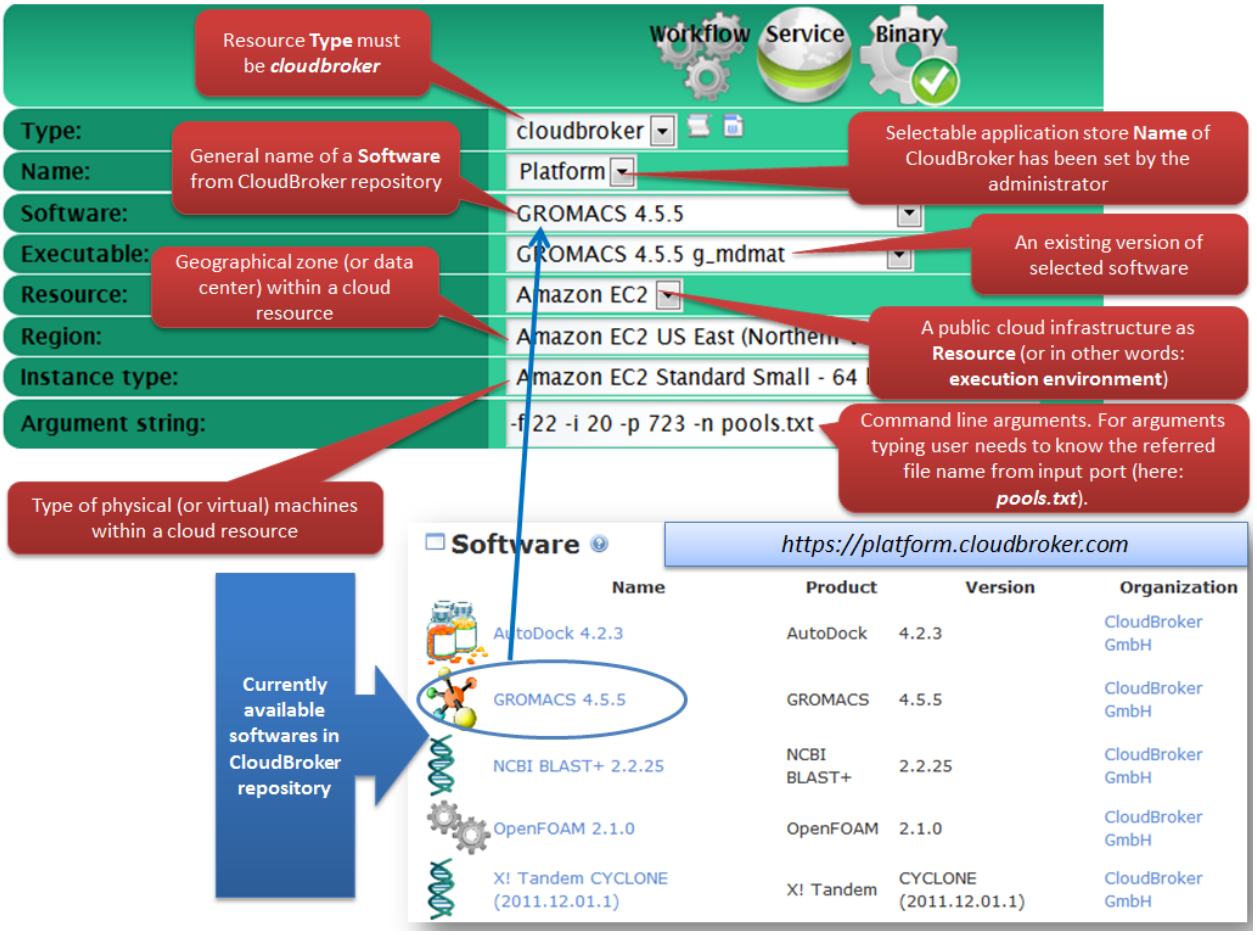
Appendix Figure 17.1 The Authentication window for CloudBroker

17.2 Configuration

The graph editing part of configuration process is the same as common configuration routine: the user can use all functions of *Graph Editor* to create nodes and connections.

The relevant novelty is found in the *Job Executable* tab of *Concrete* window within CB configuration process. (The details of settings shows figure 17.2.) The user needs to use the valid CB name (e.g. *Platform*) that set by the administrator and to that added the user his/her authentication data in the Authentication window mentioned earlier (*Security/Cloudbroker* menu: figure 17.1)

Note, that in case of *cloudbroker* resource the job interpretation is always “*Binary*”, namely the queried registered programs as jobs are binary-type programs.



Type:	cloudbroker
Name:	Platform
Software:	GROMACS 4.5.5
Executable:	GROMACS 4.5.5 g_mdmat
Resource:	Amazon EC2
Region:	Amazon EC2 US East (Northern
Instance type:	Amazon EC2 Standard Small - 64
Argument string:	-f 22 -i 20 -p 723 -n pools.txt

Resource **Type** must be ***cloudbroker***

General name of a **Software** from CloudBroker repository

Selectable application store **Name** of CloudBroker has been set by the administrator

An existing version of selected software

Geographical zone (or data center) within a cloud resource

A public cloud infrastructure as **Resource** (or in other words: **execution environment**)

Command line arguments. For arguments typing user needs to know the referred file name from input port (here: ***pools.txt***).

Type of physical (or virtual) machines within a cloud resource

Currently available softwares in CloudBroker repository

Software

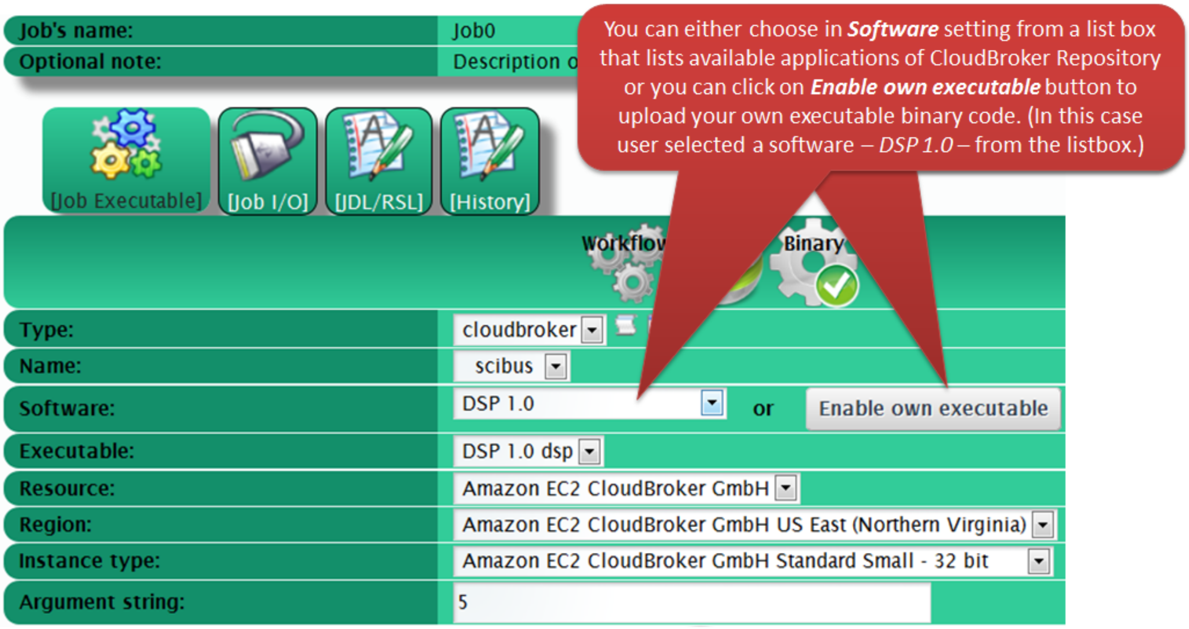
https://platform.cloudbroker.com

Name	Product	Version	Organization
AutoDock 4.2.3	AutoDock	4.2.3	CloudBroker GmbH
GROMACS 4.5.5	GROMACS	4.5.5	CloudBroker GmbH
NCBI BLAST+ 2.2.25	NCBI BLAST+	2.2.25	CloudBroker GmbH
OpenFOAM 2.1.0	OpenFOAM	2.1.0	CloudBroker GmbH
X! Tandem CYCLONE (2011.12.01.1)	X! Tandem	CYCLONE (2011.12.01.1)	CloudBroker GmbH

Appendix Figure 17.2 Sample property settings of a job in case of CloudBroker resource

There is an opportunity to use your own executable binary code in CB job configuration process beside the selection of available software from *Software list* (see Appendix Figure 17.3 and 17.4). This option is applicable by user if the corresponding *Software* and *Executable* names are earlier set to an application store (in this case to store *scibus* – as you see on next two figures) on a submission tool (e.g., DCI Bridge) by administrator.

The field of use own code is not appeared in every CB-based job configuration among other job settings in configuration window (see Appendix Figure 17.2). In order to use it, it is necessary formerly to prepare an image in a cloud and create new software that can run the user executable code over free resources defined in CB.



Job's name: Job0

Optional note: Description o

You can either choose in ***Software*** setting from a list box that lists available applications of CloudBroker Repository or you can click on ***Enable own executable*** button to upload your own executable binary code. (In this case user selected a software – *DSP 1.0* – from the listbox.)

Type: cloudbroker

Name: scibus

Software: DSP 1.0

Executable: DSP 1.0 dsp

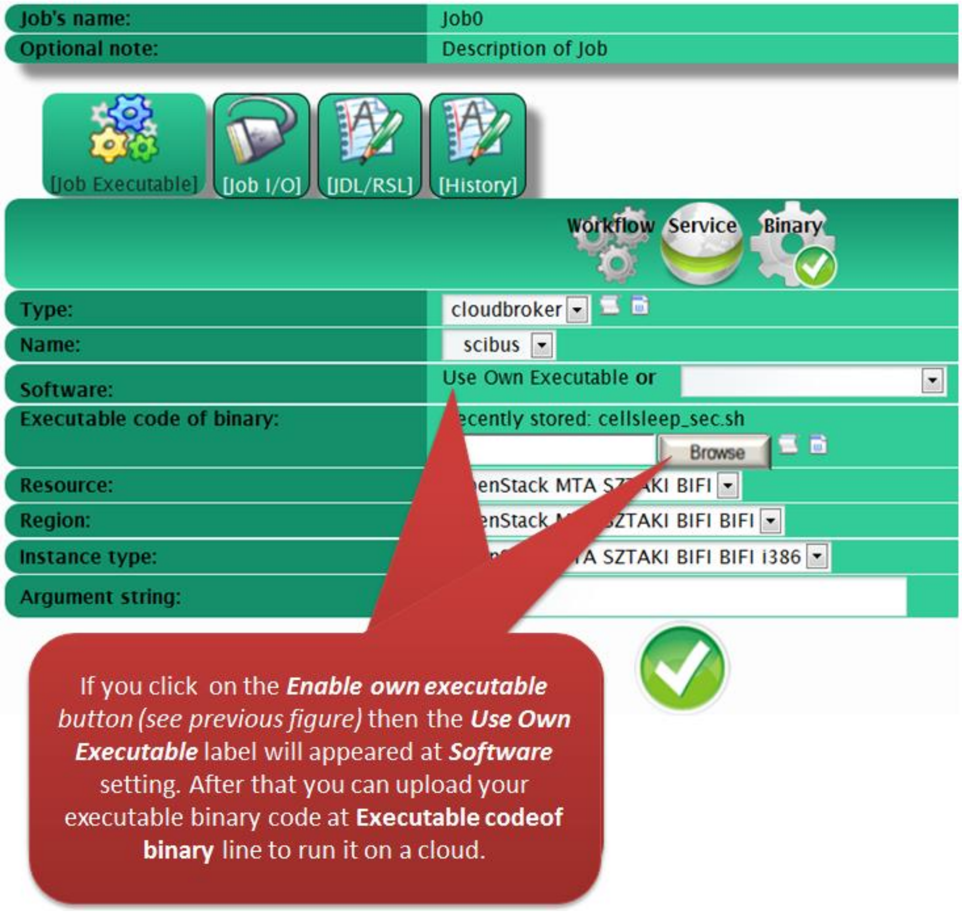
Resource: Amazon EC2 CloudBroker GmbH

Region: Amazon EC2 CloudBroker GmbH US East (Northern Virginia)

Instance type: Amazon EC2 CloudBroker GmbH Standard Small - 32 bit

Argument string: 5

Appendix Figure 17.3 There are two alternatives to run executable in cloud by CloudBroker: the using of software list of CloudBroker Repository or using of own binary code from local machine



Job's name: Job0

Optional note: Description of Job

Type: cloudbroker

Name: scibus

Software: Use Own Executable or

Executable code of binary: ecently stored: cellsleep_sec.sh

Resource: enStack MTA S KI BIFI

Region: enStack M ZTAKI BIFI BIFI

Instance type: A SZTAKI BIFI BIFI i386

Argument string:

If you click on the ***Enable own executable*** button *(see previous figure)* then the ***Use Own Executable*** label will appeared at ***Software*** setting. After that you can upload your executable binary code at **Executable codeof binary** line to run it on a cloud.

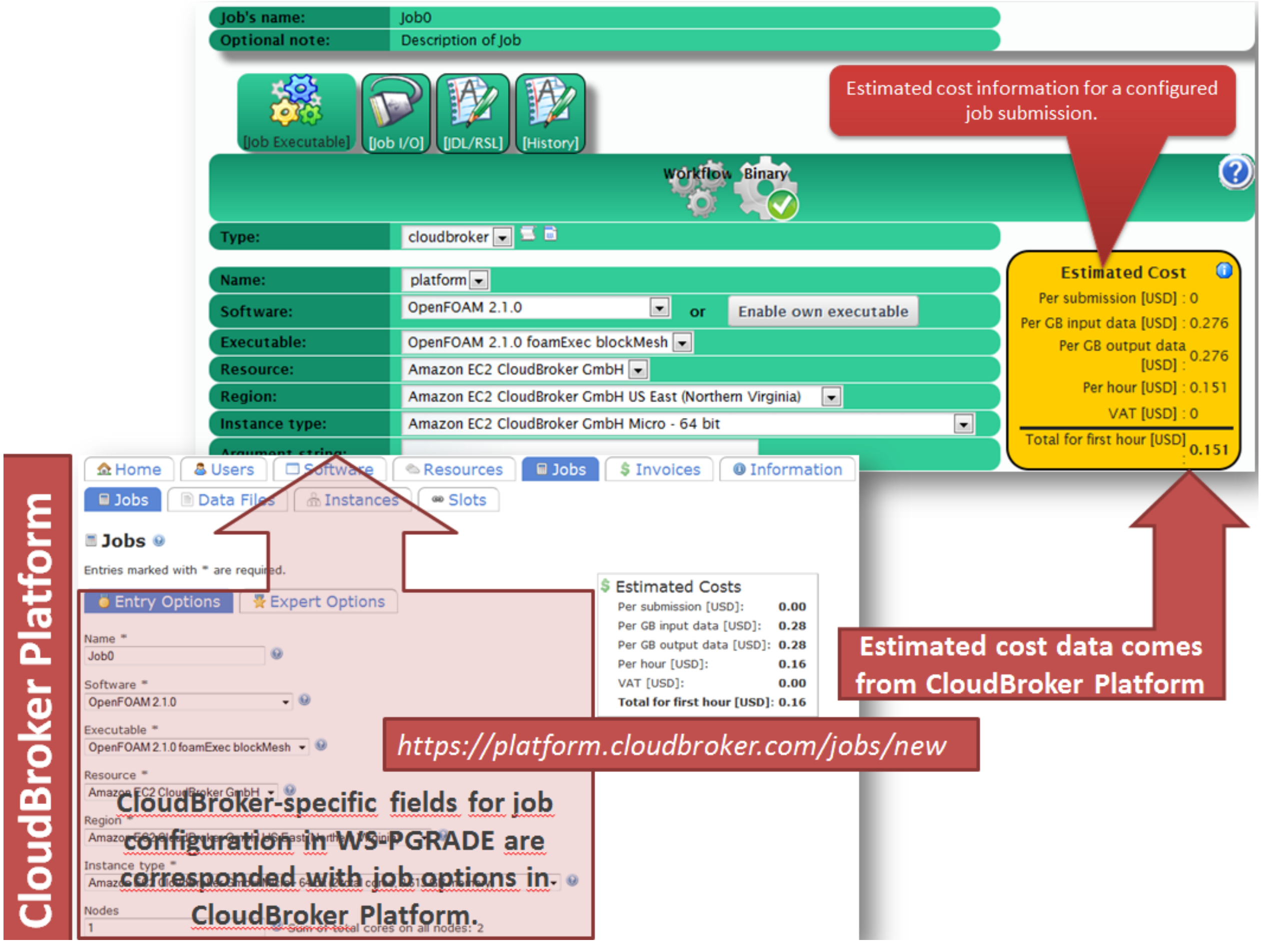
Appendix Figure 17.4 The option of use own executable on CloudBroker-based job configuration

Since the CB Platform is a pay-per-use service, WS-PGRADE provides cost information to users. The configuration side of WS-PGRADE provided cost information containing the followings (to access overall information about billing and pricing data, WS-PGRADE provides the *CloudBroker Billing* menu – see chapter 17.2):

- Information about estimated cost of a job submission in Workflow/Concrete/Configure/Job Executable function (see Appendix Figure 17.5).
- Information about cloud storage usage cost of a job in Workflow/Concrete/Configure/Job I/O function (see Appendix Figure 17.6).
- Information about aggregate estimated costs of CB-specific jobs in a workflow in Workflow/Concrete/Configure function (see Appendix Figure 17.7).
- Information about cost of submitted job instance (see Appendix Figure 17.8).

Note: the costs calculated in WS-PGRADE are only estimates, assuming one CPU hour execution, and one instance per job. Costs of storages, costs of PS job executions (more than one instances per job) and jobs running longer than one hour are not regarded. Real costs may therefore dramatically exceed the estimated costs.

The indicated cost data based on CB Platform is updated in every 30 seconds in WS-PGRADE.



Job's name: Job0
Optional note: Description of Job
Type: cloudbroker
Name: platform
Software: OpenFOAM 2.1.0 or
Executable: OpenFOAM 2.1.0 foamExec blockMesh
Resource: Amazon EC2 CloudBroker GmbH
Region: Amazon EC2 CloudBroker GmbH US East (Northern Virginia)
Instance type: Amazon EC2 CloudBroker GmbH Micro - 64 bit
Argument string:

Estimated cost information for a configured job submission.

Estimated Cost

Per submission [USD] :	0
Per GB input data [USD] :	0.276
Per GB output data [USD] :	0.276
Per hour [USD] :	0.151
VAT [USD] :	0
Total for first hour [USD] :	0.151

CloudBroker Platform

Jobs

Entries marked with * are required.

Name * Job0
Software * OpenFOAM 2.1.0
Executable * OpenFOAM 2.1.0 foamExec blockMesh
Resource * Amazon EC2 CloudBroker GmbH
Region *
Instance type *
Nodes 1
Sum of total cores on all nodes: 2

Estimated Costs

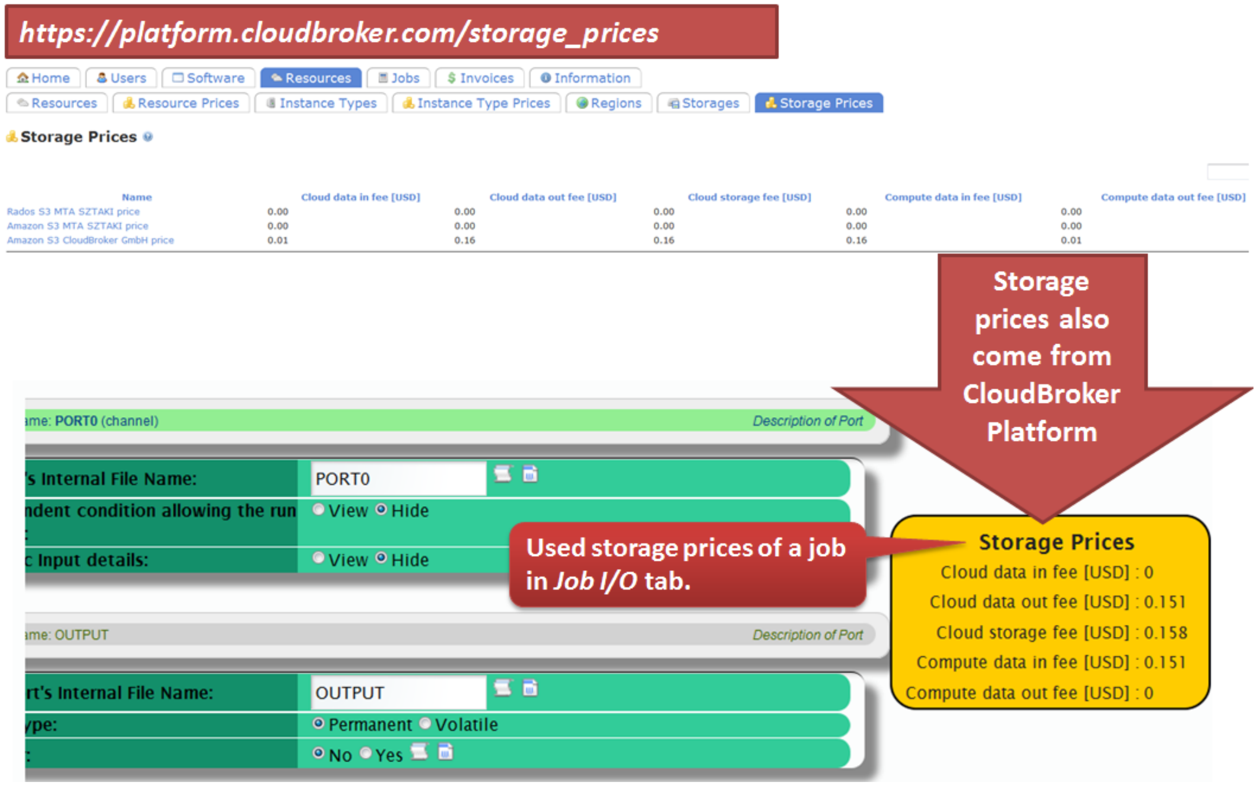
Per submission [USD]:	0.00
Per GB input data [USD]:	0.28
Per GB output data [USD]:	0.28
Per hour [USD]:	0.16
VAT [USD]:	0.00
Total for first hour [USD]:	0.16

Estimated cost data comes from CloudBroker Platform

https://platform.cloudbroker.com/jobs/new

CloudBroker-specific fields for job configuration in WS-PGRADE are corresponded with job options in CloudBroker Platform.

Appendix Figure 17.5 Providing billing information (estimated cost of a job submission) in Job Executable tab


https://platform.cloudbroker.com/storage_prices
Home
Users
Software
Resources
Jobs
Invoices
Information
Resources
Resource Prices
Instance Types
Instance Type Prices
Regions
Storages
Storage Prices

Storage Prices

Name	Cloud data in fee [USD]	Cloud data out fee [USD]	Cloud storage fee [USD]	Compute data in fee [USD]	Compute data out fee [USD]
Rados S3 MTA SZTAKI price	0.00	0.00	0.00	0.00	0.00
Amazon S3 MTA SZTAKI price	0.00	0.00	0.00	0.00	0.00
Amazon S3 CloudBroker GmbH price	0.01	0.16	0.16	0.16	0.01

Storage prices also come from CloudBroker Platform

ame: PORT0 (channel)

Description of Port

's Internal File Name: PORT0

ndent condition allowing the run: ○ View ● Hide

c Input details: ○ View ● Hide

Used storage prices of a job in *Job I/O* tab.

ame: OUTPUT

Description of Port

rt's Internal File Name: OUTPUT

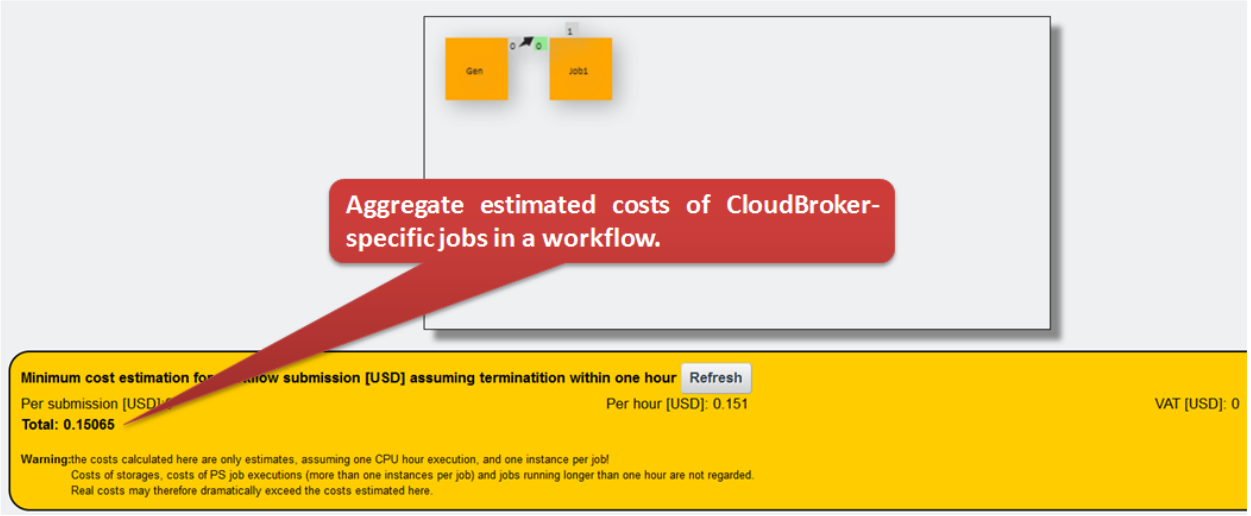
ype: ● Permanent ○ Volatile

: ● No ○ Yes

Storage Prices

Cloud data in fee [USD] : 0
Cloud data out fee [USD] : 0.151
Cloud storage fee [USD] : 0.158
Compute data in fee [USD] : 0.151
Compute data out fee [USD] : 0

Appendix Figure 17.6 Providing billing information (cloud storage usage prices of a job) in Job I/O tab


Gen
Job1
0
0
1
Refresh

Aggregate estimated costs of CloudBroker-specific jobs in a workflow.

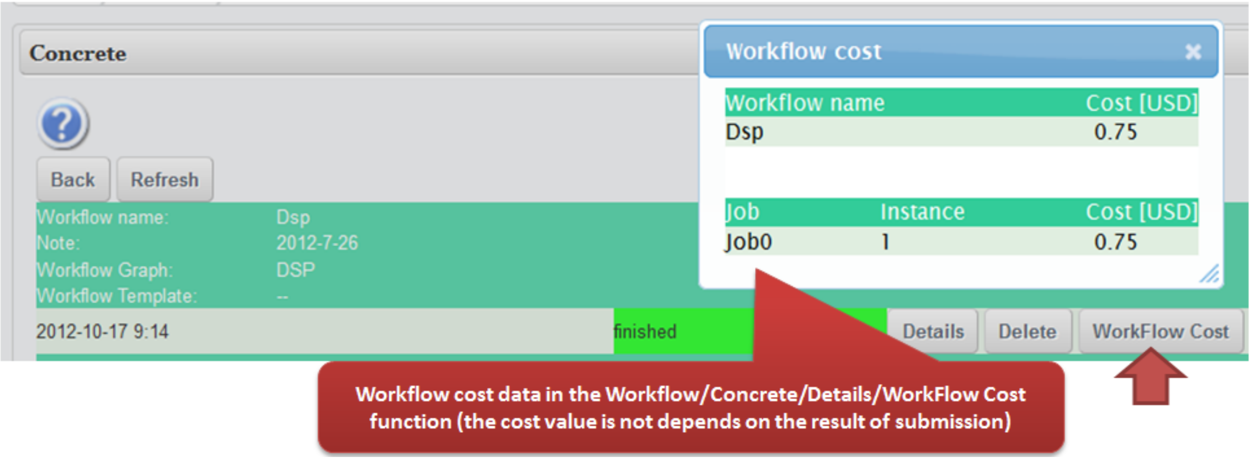
Minimum cost estimation fo ow submission [USD] assuming terminatition within one hour

Per submission [USD] Per hour [USD]: 0.151 VAT [USD]: 0

Total: 0.15065

Warning:the costs calculated here are only estimates, assuming one CPU hour execution, and one instance per job!
Costs of storages, costs of PS job executions (more than one instances per job) and jobs running longer than one hour are not regarded.
Real costs may therefore dramatically exceed the costs estimated here.

Appendix Figure 17.7 Providing billing information (aggregate estimated cost of a workflow) in Concrete/Configure function


Concrete
Back
Refresh
Details
Delete
WorkFlow Cost
Workflow cost

Workflow name: Dsp
Note: 2012-7-26
Workflow Graph: DSP
Workflow Template: --
2012-10-17 9:14 finished

Workflow name	Cost [USD]
Dsp	0.75

Job	Instance	Cost [USD]
Job0	1	0.75

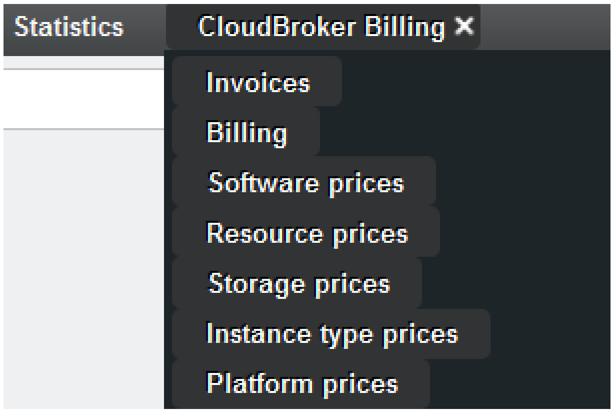
Workflow cost data in the Workflow/Concrete/Details/WorkFlow Cost function (the cost value is not depends on the result of submission)

Appendix Figure 17.8 Providing billing information (real workflow cost after submission) in Concrete/Details/Workflow Cost function

17.3 The CloudBroker Billing menu

The *CloudBroker Billing* menu provides overall billing and pricing data obtained from the CB platform through the portal interface. The *CloudBroker Billing* menu (portlet, technically) consists of the following seven submenus and functions (see Appendix Figure 17.9):

- *Invoices* - overall invoicing information for the portal user from the CB Platform.
- *Billing* - billing information for the CB Platform jobs run from the portal.
- *Software prices* - price list for software usage.
- *Resource prices* - price list for resources usage.
- *Storage prices* - price list for storage usage.
- *Instance type prices* - price list for instance type usage.
- *Platform prices* – payment plans for CB platform usage.


Statistics
CloudBroker Billing ×
Invoices
Billing
Software prices
Resource prices
Storage prices
Instance type prices
Platform prices

Appendix Figure 17.9 The *CloudBroker Billing* menu

Note: For correct usage of these functions, the following prerequisites should be met:

At least one CloudBroker platform instantiation shall be enabled under the DCI Bridge. To do so, under the DCI Bridge configuration page (you can access it through *Information/Resources* menu) select the *Cloudbroker* tab in the menu and then click on the *Add new* link. Fill in all the required fields and save your changes. To edit or view your existing CB platform instantiations, click on the *Edit* link.

The correct CB platform user authentication credentials shall be given on the portal side under the *Security/CloudBroker*.

The detailed functions of submenus:

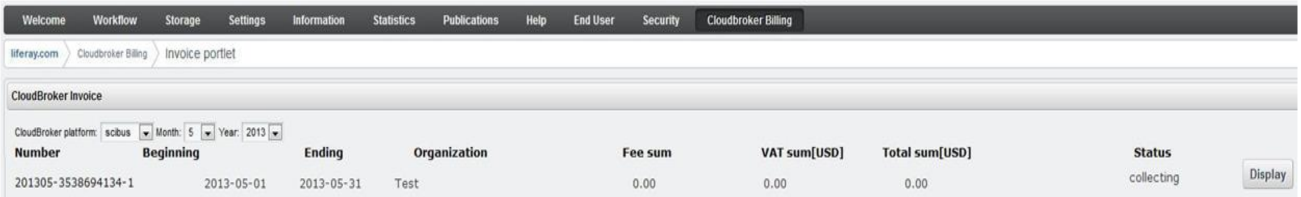
***Invoices* menu (Appendix Figure 17.10)**: it gives an overview of the overall portal user costs and expenses within the CB Platform. A new invoice is generated on the first day of the each month and comprises not only all job-related fees of a certain user (i.e. the information from the *Billing* portlet), but all other costs and expenses incurred by the CB platform usage. On the left top of the page there are three dropdown filters:

- *Cloudbroker platform* for selecting the CBP instantiation to work with,
- *Month* and
- *Year* for selecting the month and the year to display the invoices for.

For each invoice there exist the following parameters:

- *Number:* the invoice number within the CB platform.
- *Beginning*: the starting date of the invoice.
- *Ending*: the ending date of the invoice.
- *Organization*: which organization the invoice is applied to.
- *Fee sum*: the sum of all fees/costs within the invoice in USD.
- *VAT sum*: the VAT amount applied to this invoice in USD.
- *Total sum*, i.e. the total invoice amount in USD that includes the fee sum and the VAT sum.
- *Status*: the current status of the invoice (*closed* If already paid, *open* if is to be paid, *collecting* if the month is still in progress).

In order to access the detailed invoice view, click on *Display* button in front of the invoice record of interest.



CloudBroker platform: scibus Month: 5 Year: 2013

Number	Beginning	Ending	Organization	Fee sum	VAT sum[USD]	Total sum[USD]	Status
201305-3538694134-1	2013-05-01	2013-05-31	Test	0.00	0.00	0.00	collecting

Appendix Figure 17.10 The *CloudBroker Billing/Invoice* function

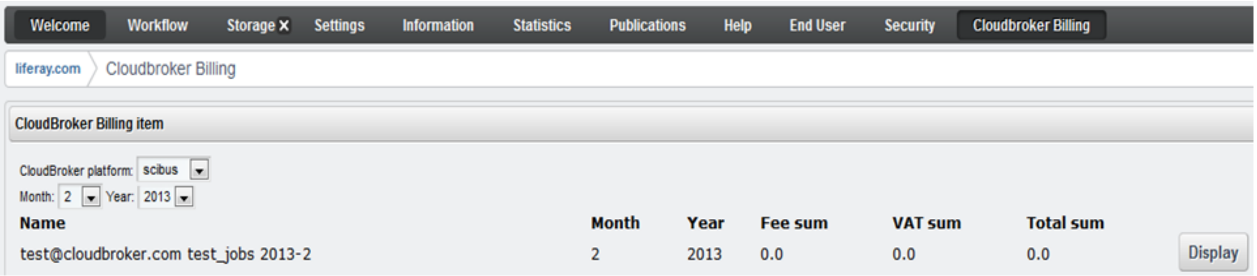
Billing menu (Appendix Figure 17.11): it provides billing information for the jobs that have been run from the portal side within the CB platform. Each billing item comprises all job-related fees for a certain user, such as jobs running or data file uploading/downloading (e.g., software license fee, cloud data in fee, compute runtime fee etc.).

On the left top of the page there are three dropdown filters: *Cloudbroker platform* for selecting the CB Platform instantiation to work with, *Month* and *Year* for selecting the month and the year to display the billing items for.

For each billing item there exist the following parameters:

- *Name*: the name of the billing item.
- *Fee sum*: the sum of all fees/costs within the billing item in USD.
- *VAT sum*: the VAT amount applied to this billing item in USD.
- *Total sum*: the total billing item amount in USD that includes the fee sum and the VAT sum.

In order to access the detailed billing item view, click on *Display* button.



CloudBroker platform: scibus
Month: 2 Year: 2013

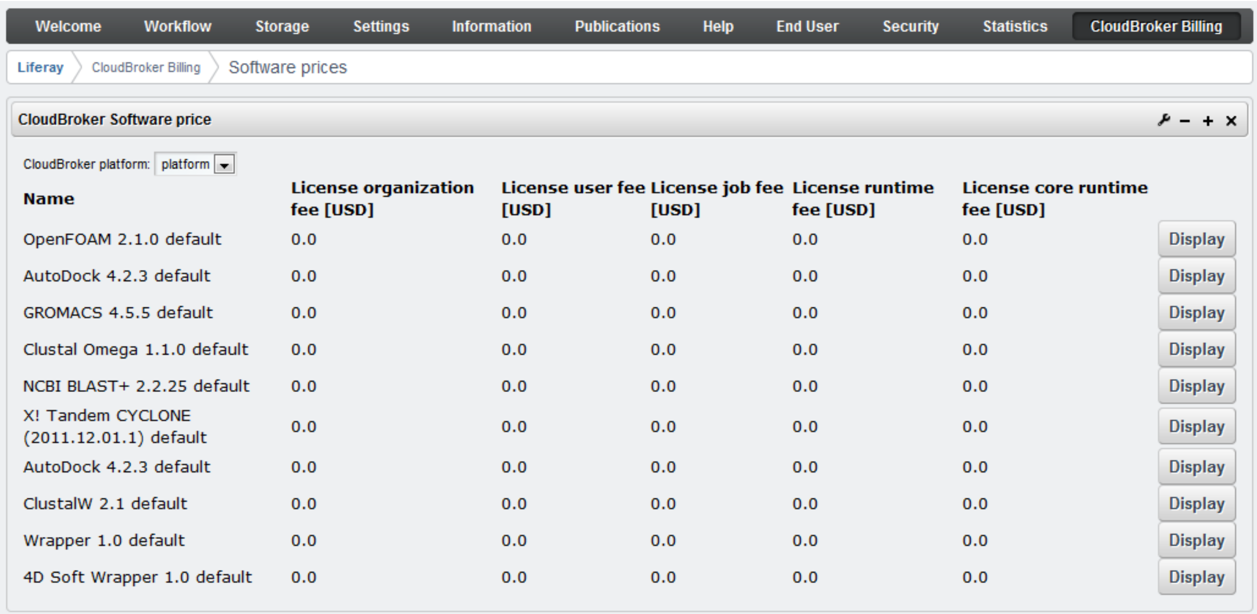
Name	Month	Year	Fee sum	VAT sum	Total sum
test@cloudbroker.com test_jobs 2013-2	2	2013	0.0	0.0	0.0

Appendix Figure 17.11 The *CloudBroker Billing/Billing* function

Software prices (Appendix Figure 17.12): it gives the information on the software pricing for the selected CB platform instantiation. For each software price there exist the following parameters:

- *Name*: the name of the software price
- *License organization fee*: the software license price per organization per month in USD.
- *License user fee*: the software license price per user per month in USD.
- License job fee: the software license price per job in USD.
- *License runtime fee*: the software license price per job runtime per hour in USD.
- *License core runtime fee*: the software license price per job runtime times the number of cores per hour in USD.

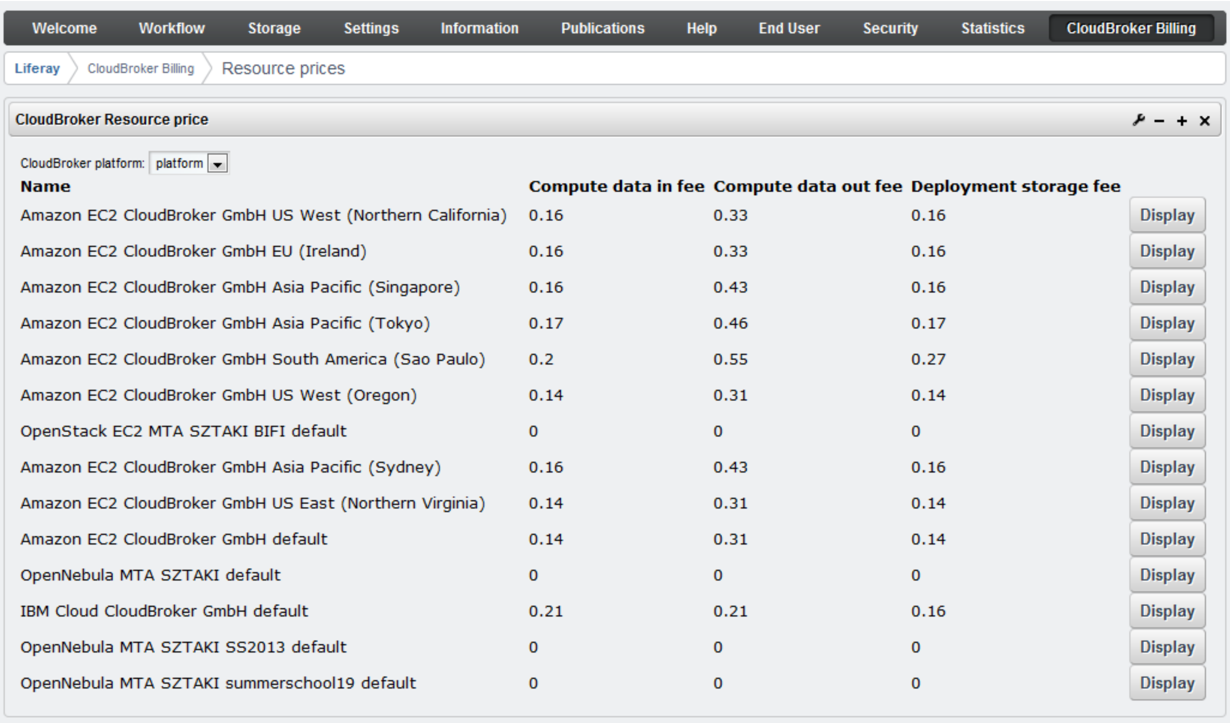
In order to access the detailed price view, click on *Display* button.


Welcome
Workflow
Storage
Settings
Information
Publications
Help
End User
Security
Statistics
CloudBroker Billing
Liferay
CloudBroker Billing
Software prices
CloudBroker Software price

CloudBroker platform: platform

Name	License organization fee [USD]	License user fee [USD]	License job fee [USD]	License runtime fee [USD]	License core runtime fee [USD]	
OpenFOAM 2.1.0 default	0.0	0.0	0.0	0.0	0.0	Display
AutoDock 4.2.3 default	0.0	0.0	0.0	0.0	0.0	Display
GROMACS 4.5.5 default	0.0	0.0	0.0	0.0	0.0	Display
Clustal Omega 1.1.0 default	0.0	0.0	0.0	0.0	0.0	Display
NCBI BLAST+ 2.2.25 default	0.0	0.0	0.0	0.0	0.0	Display
X! Tandem CYCLONE (2011.12.01.1) default	0.0	0.0	0.0	0.0	0.0	Display
AutoDock 4.2.3 default	0.0	0.0	0.0	0.0	0.0	Display
ClustalW 2.1 default	0.0	0.0	0.0	0.0	0.0	Display
Wrapper 1.0 default	0.0	0.0	0.0	0.0	0.0	Display
4D Soft Wrapper 1.0 default	0.0	0.0	0.0	0.0	0.0	Display

Appendix Figure 17.12 The *CloudBroker Billing/Software prices* function


Welcome
Workflow
Storage
Settings
Information
Publications
Help
End User
Security
Statistics
CloudBroker Billing
Liferay
CloudBroker Billing
Resource prices
CloudBroker Resource price

CloudBroker platform: platform

Name	Compute data in fee	Compute data out fee	Deployment storage fee	
Amazon EC2 CloudBroker GmbH US West (Northern California)	0.16	0.33	0.16	Display
Amazon EC2 CloudBroker GmbH EU (Ireland)	0.16	0.33	0.16	Display
Amazon EC2 CloudBroker GmbH Asia Pacific (Singapore)	0.16	0.43	0.16	Display
Amazon EC2 CloudBroker GmbH Asia Pacific (Tokyo)	0.17	0.46	0.17	Display
Amazon EC2 CloudBroker GmbH South America (Sao Paulo)	0.2	0.55	0.27	Display
Amazon EC2 CloudBroker GmbH US West (Oregon)	0.14	0.31	0.14	Display
OpenStack EC2 MTA SZTAKI BIFI default	0	0	0	Display
Amazon EC2 CloudBroker GmbH Asia Pacific (Sydney)	0.16	0.43	0.16	Display
Amazon EC2 CloudBroker GmbH US East (Northern Virginia)	0.14	0.31	0.14	Display
Amazon EC2 CloudBroker GmbH default	0.14	0.31	0.14	Display
OpenNebula MTA SZTAKI default	0	0	0	Display
IBM Cloud CloudBroker GmbH default	0.21	0.21	0.16	Display
OpenNebula MTA SZTAKI SS2013 default	0	0	0	Display
OpenNebula MTA SZTAKI summerschool19 default	0	0	0	Display

Appendix Figure 17.13 The *CloudBroker Billing/Resource prices* function

Resource prices (Appendix Figure 17.13): it gives the information on the resource pricing for the selected CB platform instantiation that can be selected on the top left corner of the page.

For each resource price there exist the following parameters:

- *Name*: the name of the resource price.
- *Compute data in fee*: the price for uploading the data files onto the virtual machine instance (in USD per GB).
- *Compute data out fee*: the price for downloading the data files from the virtual machine instance (in USD per GB).
- *Deployment storage fee*: the price for storing the virtual image (in USD per GB per month).

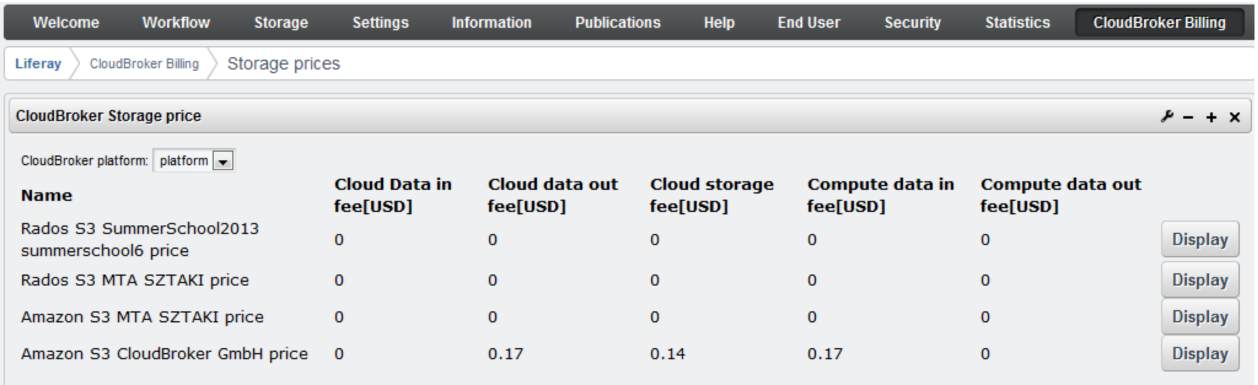
In order to access the detailed price view, click on *Display* button.

Storage prices (Appendix Figure 17.14): it gives information on the storage pricing for the selected CB platform instantiation.

For each storage price there exist the following parameters:

- *Name*: the name of the storage price.
- *Cloud data in fee*: the price for uploading the data files onto the persistent storage (in USD per GB).
- *Cloud data out fee*: the price for downloading the data files from the persistent storage (in USD per GB).
- *Cloud storage fee*: the price for storing the data (in USD per GB per month).
- *Compute data in fee*: the price for uploading the data files from the persistent storage into the virtual machine instance (in USD per GB).
- *Compute data out fee*: the price for downloading the data files from the virtual machine instance into the persistent storage (in USD per GB).

In order to access the detailed price view, click on *Display* button.



CloudBroker platform: platform

Name	Cloud Data in fee[USD]	Cloud data out fee[USD]	Cloud storage fee[USD]	Compute data in fee[USD]	Compute data out fee[USD]	
Rados S3 SummerSchool2013 summerschool6 price	0	0	0	0	0	Display
Rados S3 MTA SZTAKI price	0	0	0	0	0	Display
Amazon S3 MTA SZTAKI price	0	0	0	0	0	Display
Amazon S3 CloudBroker GmbH price	0	0.17	0.14	0.17	0	Display

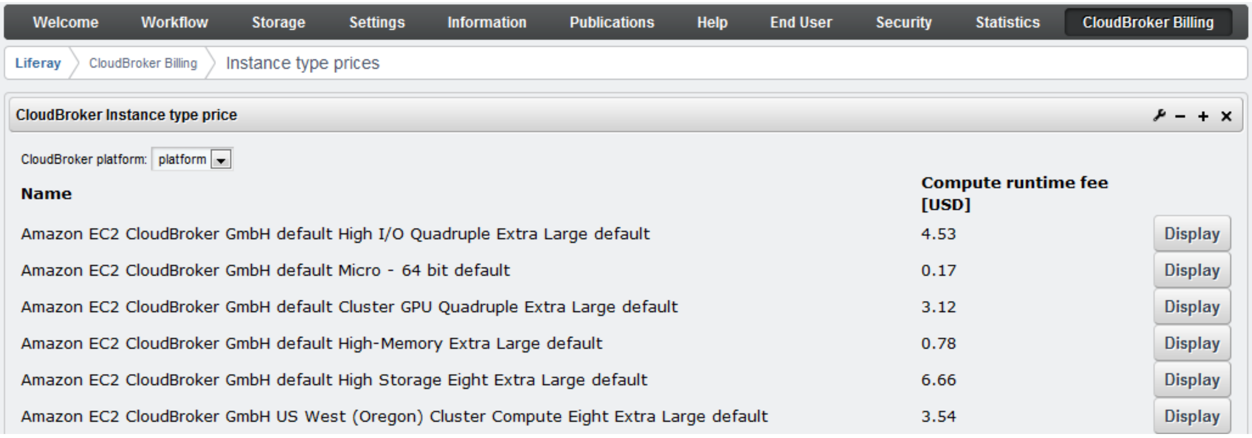
Appendix Figure 17.14 The *CloudBroker Billing/Storage prices* function

Instance type prices (Appendix Figure 17.15): it gives information on the virtual machine instances pricing for the selected CB platform instantiation.

For each instance type price there exist the following parameters:

- *Name*: the name of the instance type price.
- *Compute runtime fee*: the price for the virtual machine instance runtime per hour in USD.

In order to access the detailed price view, click on *Display*.


Welcome
Workflow
Storage
Settings
Information
Publications
Help
End User
Security
Statistics
CloudBroker Billing
Liferay
CloudBroker Billing
Instance type prices
CloudBroker Instance type price
CloudBroker platform:
platform

Name	Compute runtime fee [USD]	
Amazon EC2 CloudBroker GmbH default High I/O Quadruple Extra Large default	4.53	Display
Amazon EC2 CloudBroker GmbH default Micro - 64 bit default	0.17	Display
Amazon EC2 CloudBroker GmbH default Cluster GPU Quadruple Extra Large default	3.12	Display
Amazon EC2 CloudBroker GmbH default High-Memory Extra Large default	0.78	Display
Amazon EC2 CloudBroker GmbH default High Storage Eight Extra Large default	6.66	Display
Amazon EC2 CloudBroker GmbH US West (Oregon) Cluster Compute Eight Extra Large default	3.54	Display

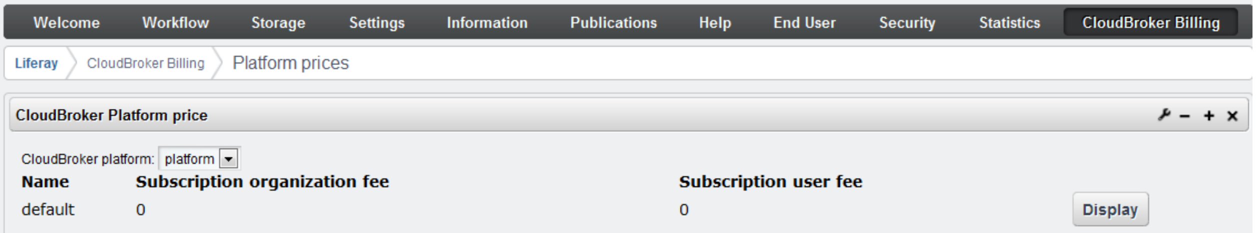
Appendix Figure 17.15 The CloudBroker Billing/Instance type prices function

Platform prices (Appendix Figure 17.16): it gives the information on the payment plan applied to the organization of the logged in portal user within the CB platform.

For each platform price there exist the following parameters:

- *Name*: the name of the CB platform.
- *Subscription organization fee*: monthly fee in USD for the given organization.
- *Subscription user fee*: monthly fee in USD for each user within the given organization.

In order to access the detailed price view, click on the *Display* button.


Welcome
Workflow
Storage
Settings
Information
Publications
Help
End User
Security
Statistics
CloudBroker Billing
Liferay
CloudBroker Billing
Platform prices
CloudBroker Platform price
CloudBroker platform:
platform

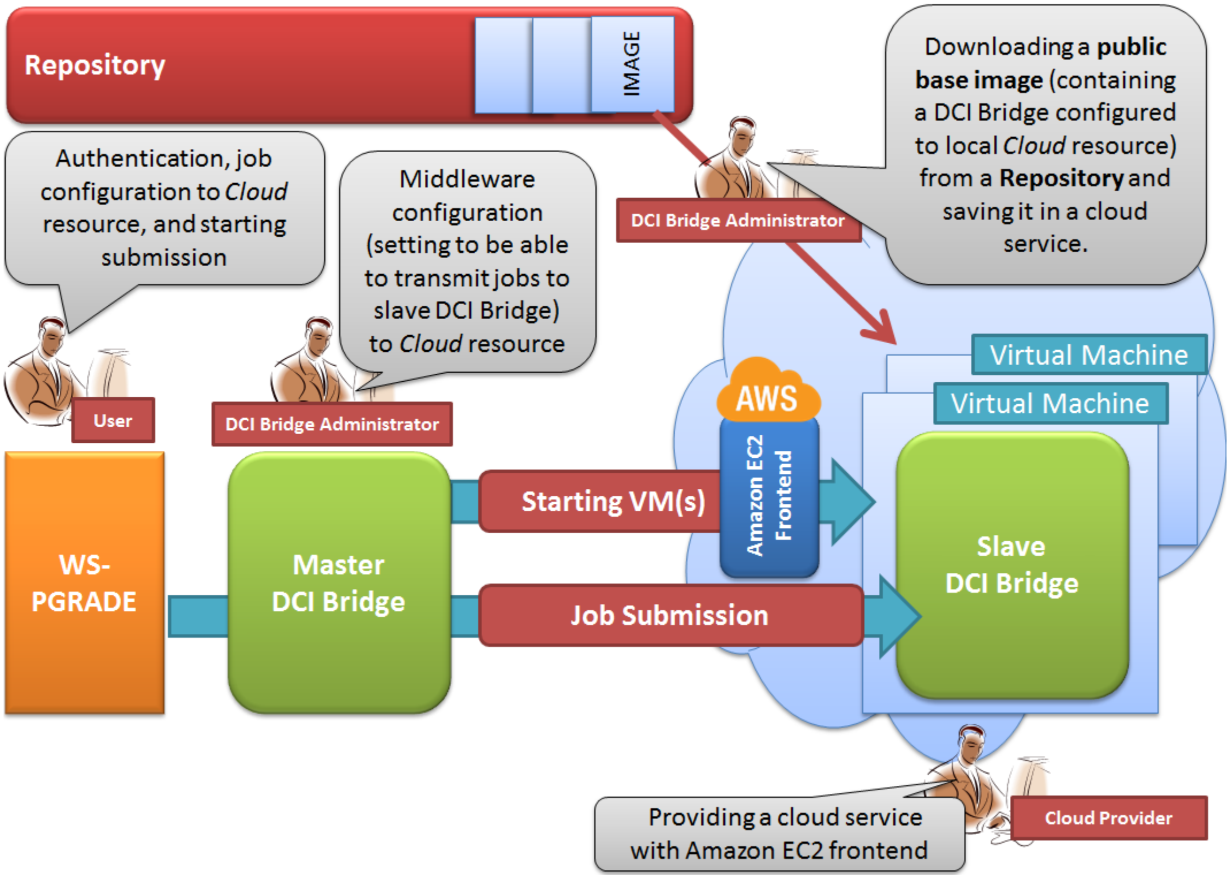
Name	Subscription organization fee	Subscription user fee	
default	0	0	Display

Appendix Figure 17.16 The *CloudBroker Billing/Platform prices* function

18. Job Submission to Cloud by EC2-based Cloud Access Solution

The chapter 17 contains details about the using of WS-PGRADE portal for job submission to cloud through a brokering platform (CloudBroker Platform, CBP).

The **EC2-based Direct Cloud Access** solution doesn't use any brokering platform for job submission to cloud. Any clouds that implements the **Amazon EC2** interface will be accessible by this development. This solution results in less administrative settings and faster job submission processes than via CBP. You can connect your gateway directly with your private cloud without any registration at CBP and in the clouds.


Repository
IMAGE
Downloading a public base image (containing a DCI Bridge configured to local Cloud resource) from a Repository and saving it in a cloud service.
DCI Bridge Administrator
Authentication, job configuration to Cloud resource, and starting submission
Middleware configuration (setting to be able to transmit jobs to slave DCI Bridge) to Cloud resource
User
DCI Bridge Administrator
WS-PGRADE
Master DCI Bridge
Starting VM(s)
Job Submission
AWS
Amazon EC2 Frontend
Virtual Machine
Virtual Machine
Slave DCI Bridge
Providing a cloud service with Amazon EC2 frontend
Cloud Provider

Appendix Figure 18.1 Overview of the EC2-based direct cloud access process

The EC2-based direct cloud access process contains the next tasks and relates the next roles (see Figure 18.1):

- **Task 1**: The DCI Bridge Administrator downloads a public base image containing a properly configured DCI Bridge (this will be the slave DCI Bridge) from a corresponding Repository. This image will be saved in the target cloud environment. (The used cloud service provided by the Cloud Provider must contain Amazon EC2 Frontend.) - *see details in DCI Bridge Manual and in Admin Manual*

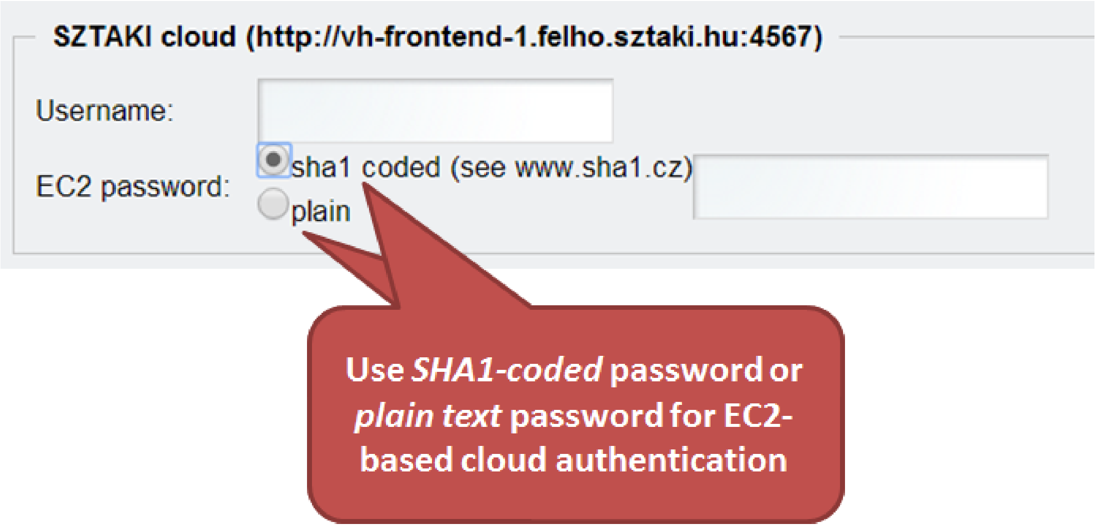
- **Task 2**: The DCI Bridge Administrator properly configures the master DCI Bridge (which connects to gUSE). - *see details in DCI Bridge Manual* and in *Admin Manual*
- **Task 3**: The WS-PGRADE User gets account from Cloud Provider to a cloud where the image was imported from the Repository (the Cloud Provider can provide information about the exact way to get cloud account). From this point the User can use the WS-PGRADE portal for job submission to cloud.

Since the **Task 3** relates to the **user-specific part** of this process, the next section describes the details of this task (see other, administration-specific task descriptions in *chapter VI* of *Admin Manual*):

User Authentication: If the user has an account to access the corresponding cloud resource, then she/he can easy use it to authenticate. Otherwise, the user previously needs to register at the Cloud provider and after registration she/he can authenticate (the Cloud provider can give information about the exact way to get cloud account).

Once the user gets authentication data (and saved it by the Save authentication), then you can use it to submit jobs. The place of user authentication to cloud is the *Security/Cloud* window (Appendix Fig. 18.2).

Note: the used password can be **in plain text** form or can be encrypted by SHA1. (For SHA1 hash code generation, see www.sha1.cz web site.)


SZTAKI cloud (http://vh-frontend-1.felho.sztaki.hu:4567)

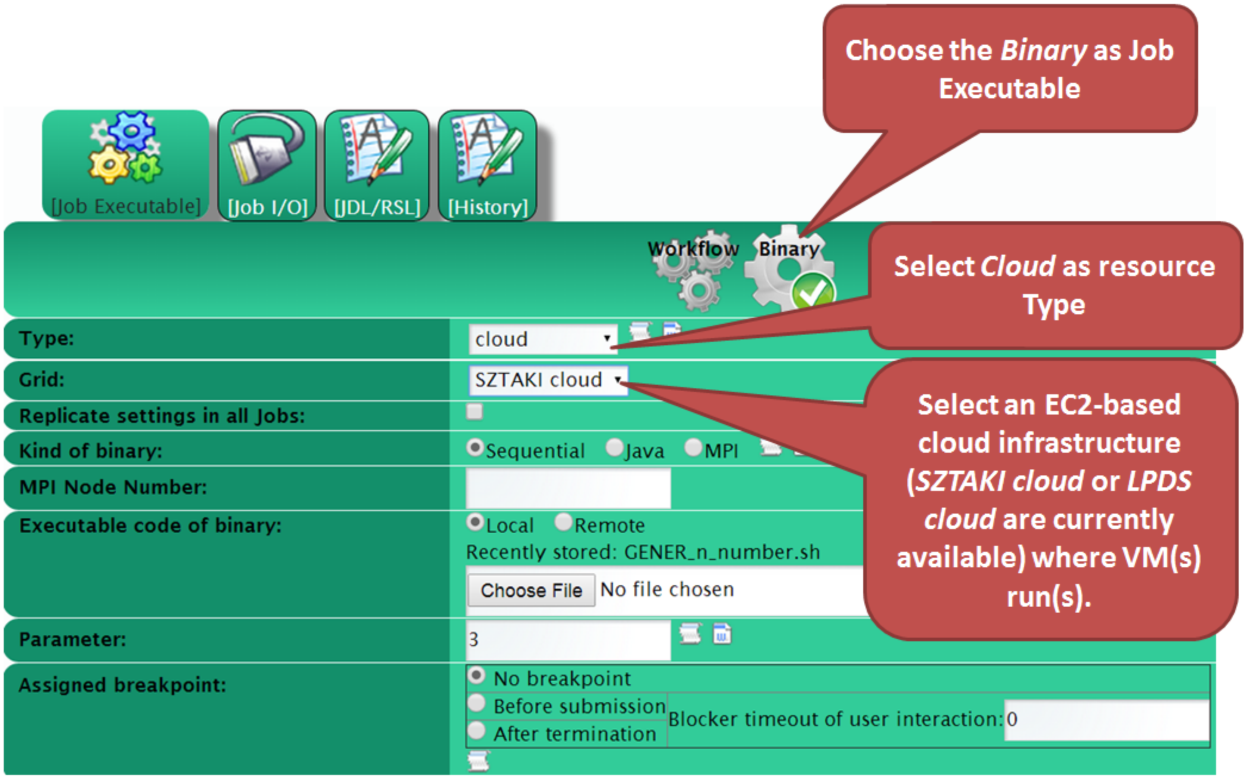
Username:

EC2 password: ● sha1 coded (see www.sha1.cz) ○ plain

Use *SHA1-coded* password or *plain text* password for EC2-based cloud authentication

Appendix Figure 18.2 User authentication to access EC2-based cloud in the *Security/Cloud* menu (the figure shows the authentication to *SZTAKI cloud*)

Job configuration: You need to sign the "*Binary*" icon on the top of the window in the *Job Executable* tab and then select the "*cloud*" at *Type* setting and "*SZTAKI cloud*" or "*LPDS cloud*" at *Grid* setting (see Appendix Fig. 18.3). The other parts of job configuration and job submission are not differing from the routine way.



Choose the *Binary* as Job Executable

Select *Cloud* as resource Type

Select an EC2-based cloud infrastructure (*SZTAKI cloud* or *LPDS cloud* are currently available) where VM(s) run(s).

Type:	cloud
Grid:	SZTAKI cloud
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	● Local ○ Remote Recently stored: GENER_n_number.sh Choose File No file chosen
Parameter:	3
Assigned breakpoint:	● No breakpoint ○ Before submission ○ After termination Blocker timeout of user interaction: 0

Appendix Figure 18.3 Job configuration

Note: To use **robot certification** for job submission, you need to do some preliminary tasks:

1. Configure your corresponding job(s) with robot certificate by adding robot permission association (about robot permission creation see chapter 20).

2. Copy the content of directory *apache-tomcat-6.0.37/temp/dci_bridge/robotcert* to the same directory of the image that contains the slave DCI Bridge (see description of *task 1* at the beginning of this chapter). About image preparation and downloading see chapter VI within Admin Manual.

3. Submit your workflow.

19. Configuration of REST Services

About REST Services

Representational State Transfer (REST) has gained widespread acceptance across the Web as a simpler alternative to SOAP- and Web Services Description Language (WSDL)-based Web services. REST defines a set of architectural principles by which you can design Web services that focus on a system's resources, including how resource states are addressed and transferred over HTTP by a wide range of clients written in different languages.

One of the key characteristics of a REST service is the explicit use of HTTP methods. HTTP GET, for instance, is defined as a data-producing method that's intended to be used by a client application to retrieve a resource, to fetch data from a Web server, or to execute a query with the expectation that the Web server will look for and respond with a set of matching resources.

The basic REST design principle establishes a one-to-one mapping between create, read, update, and delete (CRUD) operations and HTTP methods. According to this mapping:

- To create a resource on the server, use POST.
- To retrieve a resource, use GET.
- To change the state of a resource or to update it, use PUT.
- To remove or delete a resource, use DELETE.

19.1 REST Service Configuration

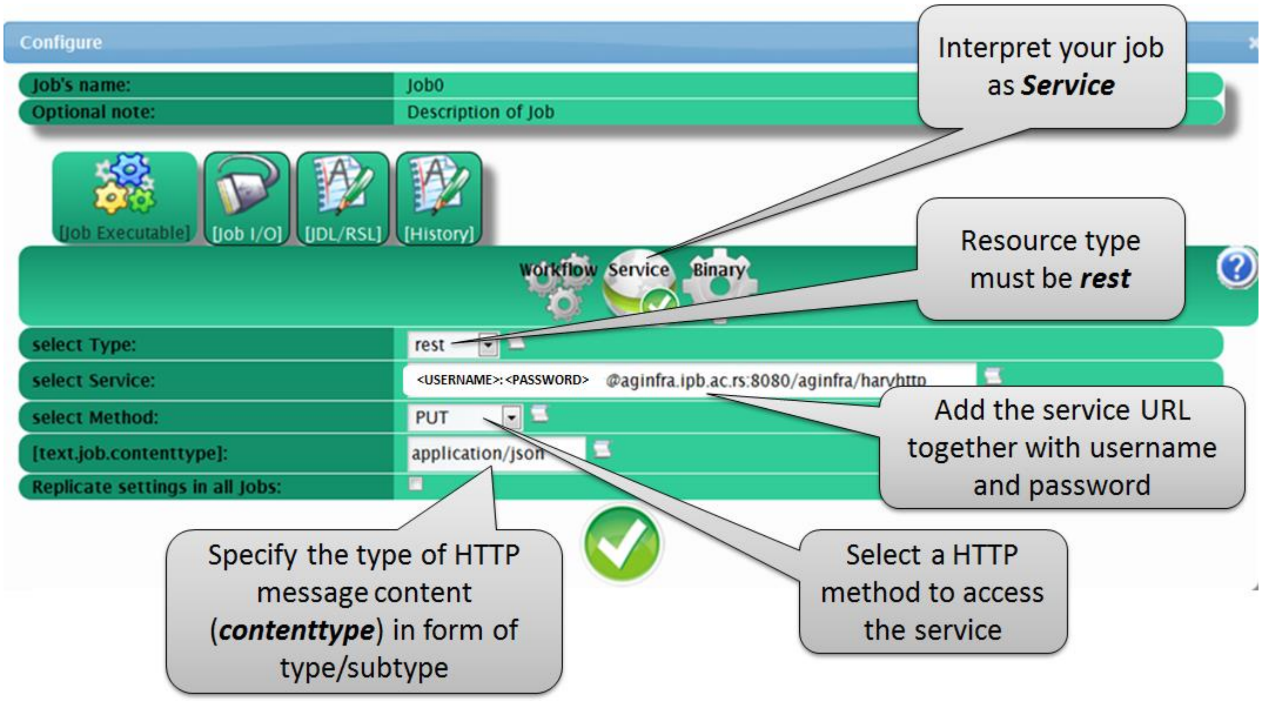
In order to configure your jobs as REST services, you need to do some special settings. The REST-specific configuration practice is related to some settings in Job Executable and Job I/O tabs within *Workflow/Concrete* function:

In *Job Executable* tab (Appendix Fig. 19.1):

- You have to interpret your job as Service.
- You need to know the exact service URL address and some other HTTP-based details: the HTTP method to access service and the HTTP message content-type for proper configuration in Job Executable tab.

In *Job I/O* tab, *Input* port (Appendix Fig. 19.2):

- You have to choose the proper HTTP sending type (the form in which data will be sent) from the three available options:
  - FORM PARAMETER: Binds the data of an HTTP request form to a key parameter.
  - URL PATH: The data of an HTTP request is added to the end of an URL address.
  - STREAM: The data of an HTTP request is added to the message body.



Job's name: Job0

Optional note: Description of Job

select Type: rest

select Service: <USERNAME>:<PASSWORD> @aginfra.ipb.ac.rs:8080/aginfra/harvhttp

select Method: PUT

[text.job.contenttype]: application/json

Replicate settings in all Jobs: ☐

Interpret your job as ***Service***

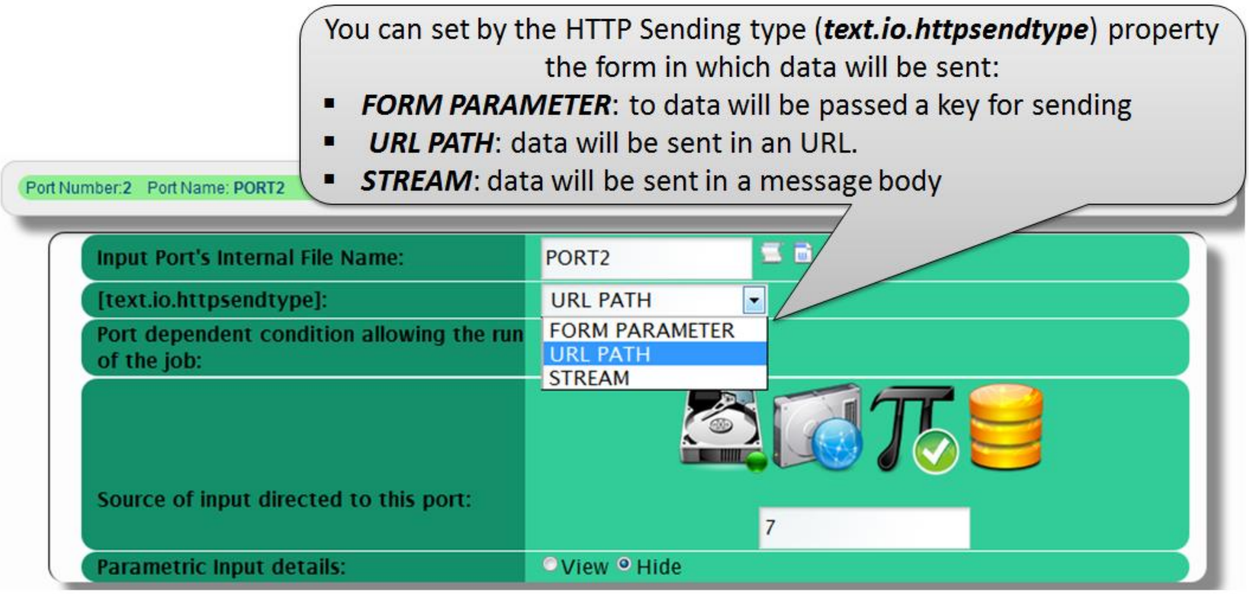
Resource type must be ***rest***

Add the service URL together with username and password

Specify the type of HTTP message content (***contenttype***) in form of type/subtype

Select a HTTP method to access the service

Appendix Figure 19.1 REST-specific job settings in Job Executable function



Port Number:2 Port Name: PORT2

Input Port's Internal File Name: PORT2

[text.io.httpsendtype]: URL PATH

Port dependent condition allowing the run of the job:

Source of input directed to this port: 7

Parametric Input details: ○ View ● Hide

You can set by the HTTP Sending type (***text.io.httpsendtype***) property the form in which data will be sent:

- ***FORM PARAMETER***: to data will be passed a key for sending
- ***URL PATH***: data will be sent in an URL.
- ***STREAM***: data will be sent in a message body

Appendix Figure 19.2 REST-specific input port settings in Job I/O function

Warnings:

Classical local file upload is only possible in STREAM-mode.

If your REST-type job needs an input file comes from a channel, then you have to use STREAM as HTTP sending type in input port configuration.

If you define a channel to run later your REST-type job than the jobs specified at the other resource side of the channel, then the input port type shouldn’t be in STREAM-mode.

20. Robot Permission Usage

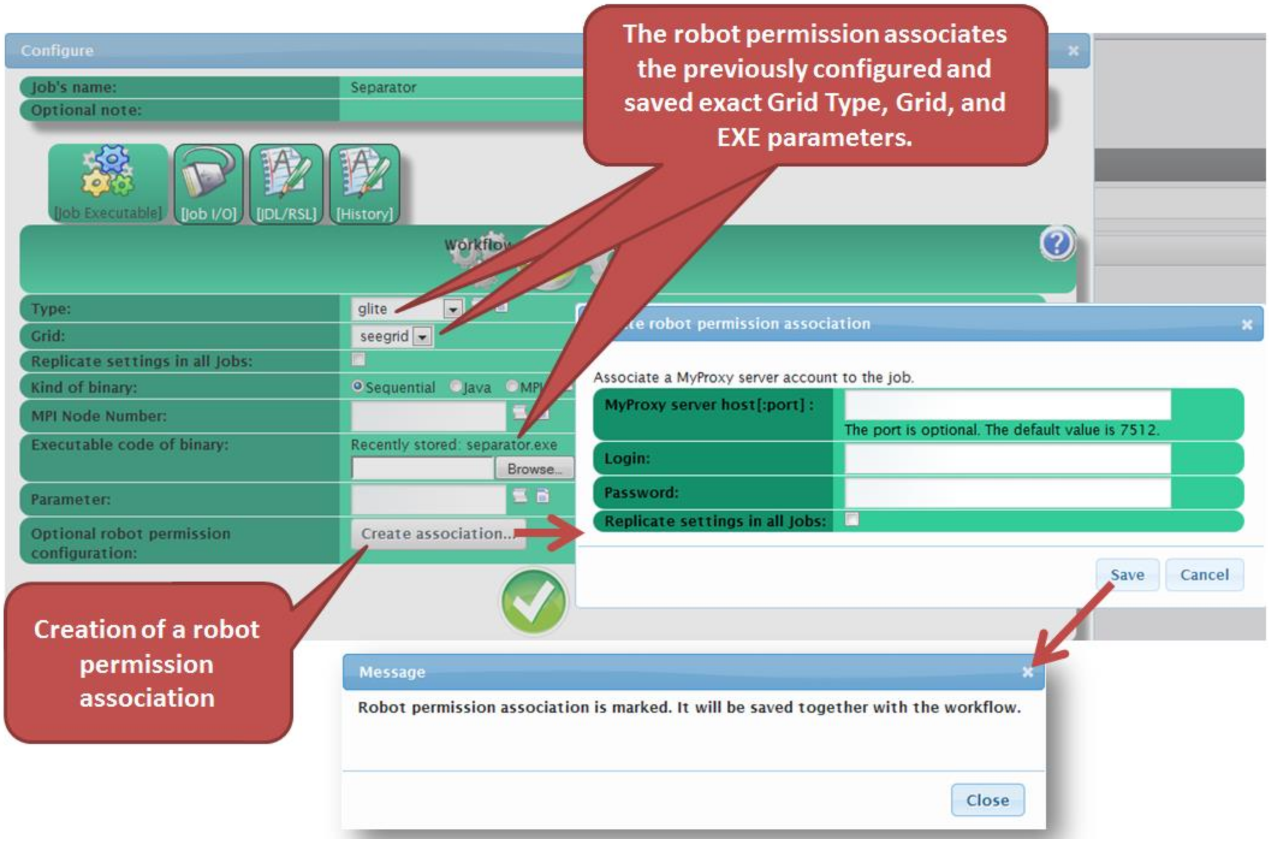
The aim in **robot permission** (or in other words **robot certification**) is to perform automated tasks on grids/clouds on behalf of users. Basically, this permission form can be used to identify a person responsible for an unattended service or process acting as client and/or server.

Instead of identifying users, the robot permission identifies trusted applications that can run by workflows from WS-PGRADE. WS-PGRADE supports robot permission for every resource type that is accessible from portal

Note: to use *local* grid type is not require robot permission.

The main advantage of robot permission is to run by user (typically end users) workflows without any direct authentication data uploading process, thus the users just needs to import/upload the previously configured and exported robot certificate-aware workflows for submissions.

Technically, the major user activity that related to settings of robot permission is in *Job Executable* tab within *Workflow/Concrete/Configure* function of WS-PGRADE.



Job's name: Separator
Optional note:
Type: glite
Grid: seegrid
Replicate settings in all Jobs: ☐
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: Recently stored: separator.exe
Parameter:
Optional robot permission configuration:

The robot permission associates the previously configured and saved exact Grid Type, Grid, and EXE parameters.

Creation of a robot permission association

…te robot permission association

Associate a MyProxy server account to the job.

MyProxy server host[:port] :
The port is optional. The default value is 7512.
Login:
Password:
Replicate settings in all Jobs: ☐

Robot permission association is marked. It will be saved together with the workflow.

Appendix Figure 20.1 Create robot permission association

The very first step in application of every robot permission association (RPA) process (after the authentication data uploading to a MyProxy server that is the same process written in the chapter 10) in WS-PGRADE is to configure jobs of a workflow (above all: setting of *Type, Grid*, and *Executable*) and then save that. (The initial submission of workflow by non-robot permission is recommended).

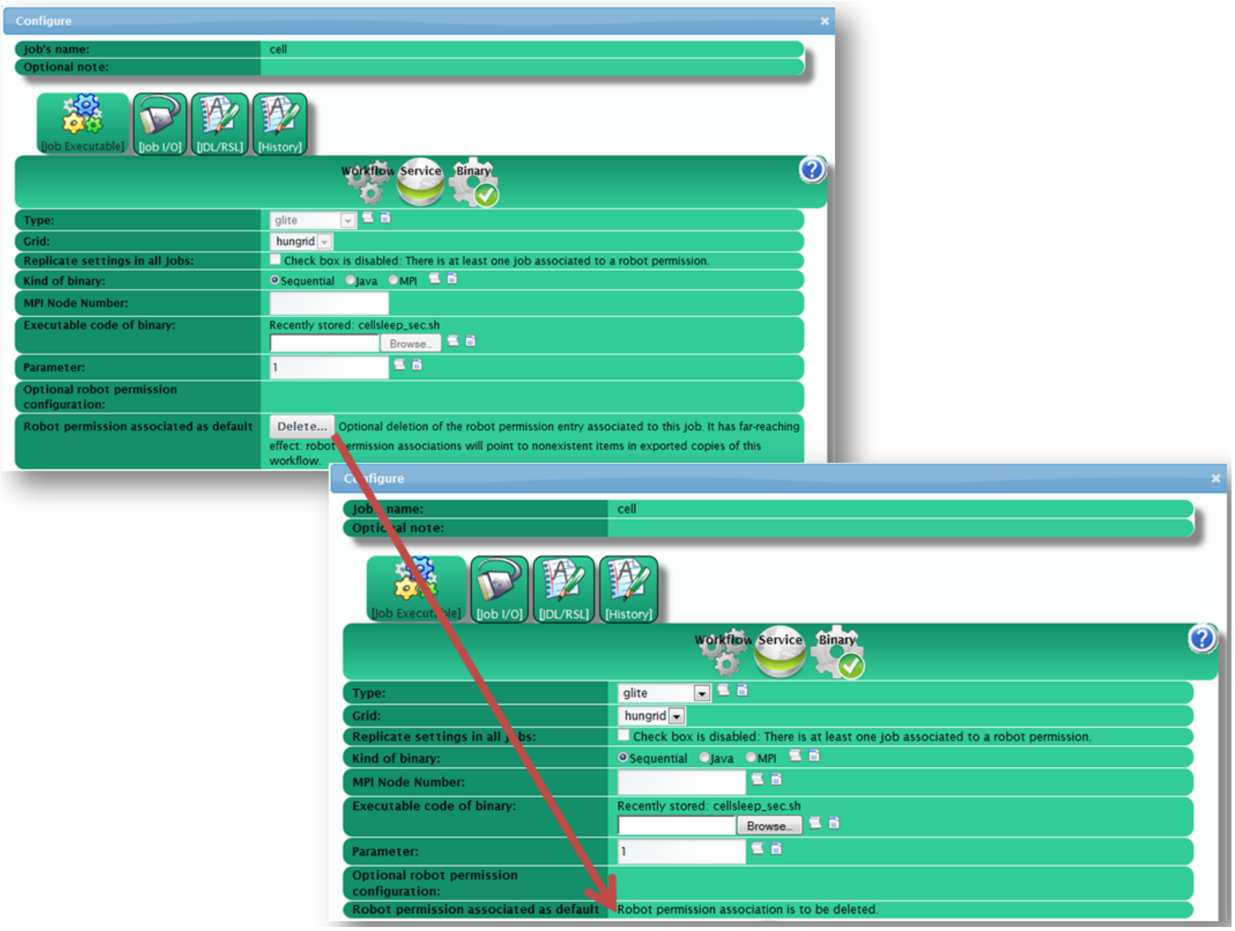
Once you saved the workflow, you can create an RPA. For RPA creation is responsible the so called **RobotPermissionOwner** (this fixed role name together with special rights are set by administrator previously), a trusted user. (For more about administration of user roles see chapter *Additional Enhancement* and chapter *IV*. in *Administrator Manual*.)

In order to create an RPA as RobotPermissionOwner click on *Create association* button in the reopened *Configure/Job Executable* tab. (Certainly, the application of RPA is always optional.) Add the well-known (you know it from WS-PGRADE Certificate function) authentication information (*MyProxy server location*, *Login*, and *Password* information). If you want to apply the current RPA setting for every job within the workflow, check the *Replicate settings in all jobs* check box. If you click on *Save*, the next message will be appeared: *Robot permission association is marked. It will be saved together with the workflow* (It is shown by the Appendix Figure 19.1). You can actually enforce this change if you save the workflow by clicking on the well-known floppy disk icon in the start-up window of workflow configuration.

You can also delete as RobotPermissionOwner the current RPA if you want to use for example the traditional certificate for job submission or if you want create another RPA. To this, click on *Delete* button in the configure window after saving the previous state of the job. (The actual change will be enforced only after the saving process.) If you open the configure page of the job, you see the next message in the last row: *Robot permission is to be deleted* (see Appendix Figure 20.2). (Note: If you delete the current association, then you delete all related data from DCI Bridge. Therefore you can create a new one if you want to apply an RPA again.)

The essential benefit of using robot permission is that other users can run without any authentication settings the applications that previously set the RobotPermissionOwner. To this the user (the permission owner or power user) need to export the robot permission-aware workflow by the traditional *Concrete/Export* function (Any portal user has rights to export this excluding end users).

In order to access any users (power users or end users) the exported workflow, you have to use *Workflow/Upload* or *Workflow/Import* function.



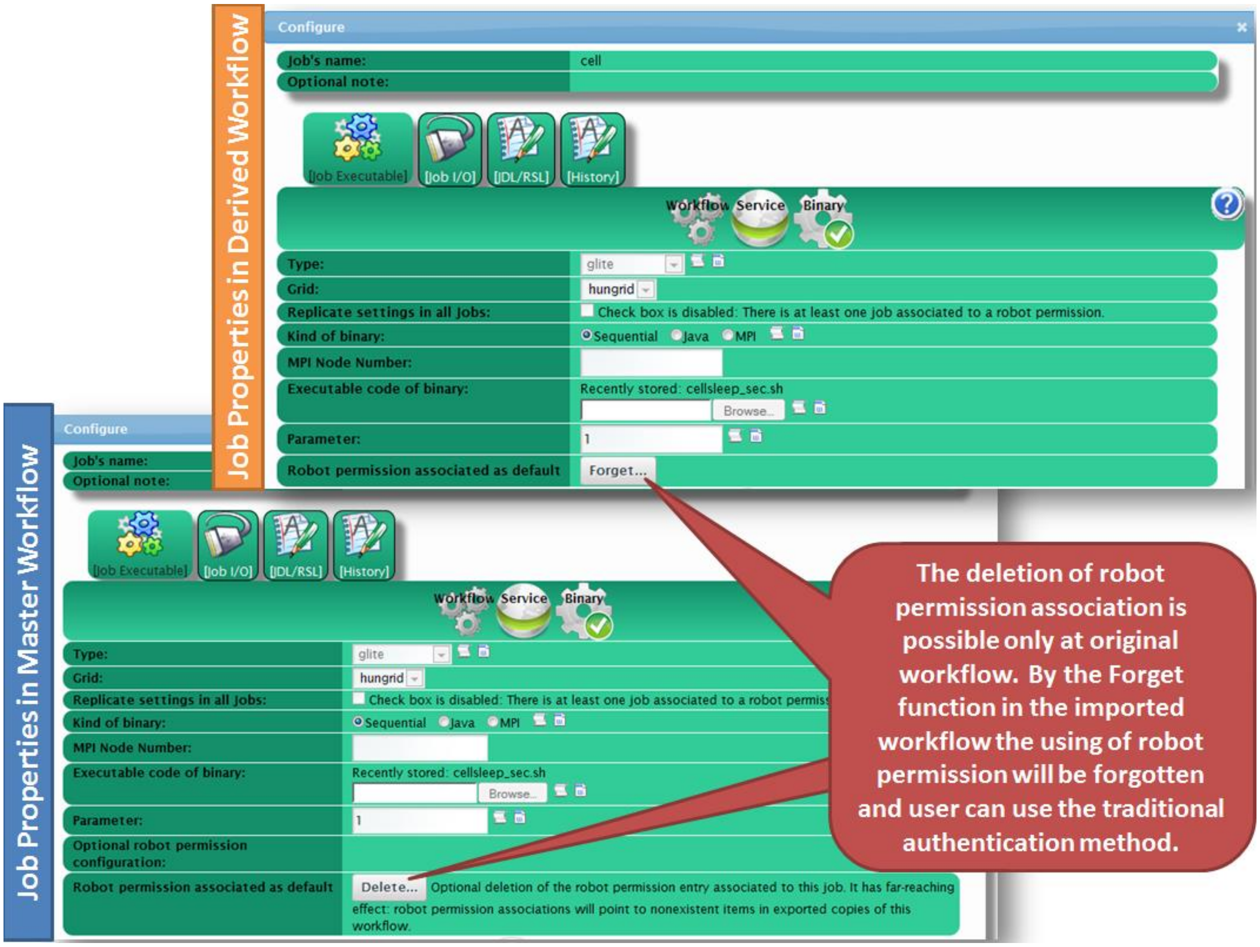
Job's name: cell
Optional note:
Type: glite
Grid: hungrid
Replicate settings in all Jobs: ☐ Check box is disabled: There is at least one job associated to a robot permission.
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: Recently stored: cellsleep_sec.sh
Parameter: 1
Optional robot permission configuration:
Robot permission associated as default: Delete... Optional deletion of the robot permission entry associated to this job. It has far-reaching effect: robot permission associations will point to nonexistent items in exported copies of this workflow.

Job's name: cell
Optional note:
Type: glite
Grid: hungrid
Replicate settings in all Jobs: ☐ Check box is disabled: There is at least one job associated to a robot permission.
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: Recently stored: cellsleep_sec.sh
Parameter: 1
Optional robot permission configuration:
Robot permission associated as default: Robot permission association is to be deleted.

Appendix Figure 20.2 Delete robot permission association

The main difference between the derived (imported or uploaded) workflow and the master (or original) workflow is that the robot permission delete function is enabled only at master workflow's job (see Appendix Figure 20.3) Therefore the robot permission owner has rights to delete RPA at master workflow. (Note, by deletion the RPA ID and the reference that points to that ID will be deleted from DCI Bridge.) If you delete an RPA from a workflow, the possibility of using this RPA is lost not only at master workflow where you deleted, but at every derived workflows too.

If you don't want to use RPA to the derived workflow, click on *Forget* button (so you avoid the using of robot permission, the RPA ID won't be deleted from DCI Bridge, only the reference that points to ID). Then use the traditional authentication method. You have also possibility to re-export the derived workflow (certainly, end user hasn't got a right for export).


Job Properties in Derived Workflow
Configure
[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Service
Binary

Job's name: cell
Optional note:
Type: glite
Grid: hungrid
Replicate settings in all jobs: ☐ Check box is disabled: There is at least one job associated to a robot permission.
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: Recently stored: cellsleep_sec.sh
Parameter: 1
Robot permission associated as default: Forget...

Job Properties in Master Workflow
Configure
[Job Executable]
[Job I/O]
[JDL/RSL]
[History]
Workflow
Service
Binary
Browse...

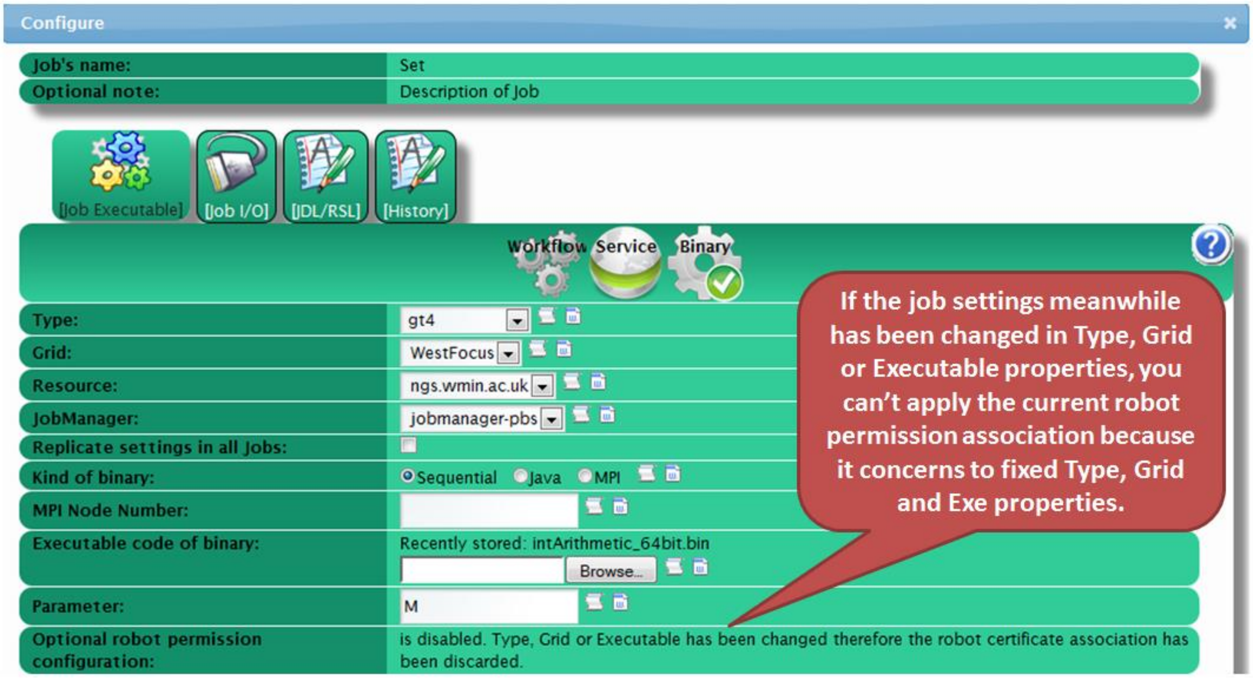
Job's name:
Optional note:
Type: glite
Grid: hungrid
Replicate settings in all jobs: ☐ Check box is disabled: There is at least one job associated to a robot permiss
Kind of binary: ● Sequential ○ Java ○ MPI
MPI Node Number:
Executable code of binary: Recently stored: cellsleep_sec.sh
Parameter: 1
Optional robot permission configuration:
Robot permission associated as default: Delete... Optional deletion of the robot permission entry associated to this job. It has far-reaching effect: robot permission associations will point to nonexistent items in exported copies of this workflow.

The deletion of robot permission association is possible only at original workflow. By the Forget function in the imported workflow the using of robot permission will be forgotten and user can use the traditional authentication method.

Appendix Figure 20.3 Difference between master and derived workflow's robot job properties

Since the RPA refers to exact grid type, grid, and exe relation, for altering the configuration you need to create another RPA. When you change at least one property from the mentioned three properties, the RPA will be discarded (see Appendix Figure 20.3). To create a new association you need to save the new job configuration settings then you can create a new RPA in the reopened Configure window.

Certainly, you can apply different grid or grid type settings for different jobs within a workflow (in this case you don't check the *Replicate settings in all jobs* check box as you can see on Appendix Figure 20.1) as well as you can add traditional or robot permissions for different jobs within a workflow too.



Job's name:	Set
Optional note:	Description of Job
Type:	gt4
Grid:	WestFocus
Resource:	ngs.wmin.ac.uk
JobManager:	jobmanager-pbs
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	Recently stored: intArithmetic_64bit.bin
Parameter:	M
Optional robot permission configuration:	is disabled. Type, Grid or Executable has been changed therefore the robot certificate association has been discarded.

If the job settings meanwhile has been changed in Type, Grid or Executable properties, you can't apply the current robot permission association because it concerns to fixed Type, Grid and Exe properties.

Appendix Figure 20.4 The job configuration settings with disabled RPA in case of changed job properties

Another important note that in a copy or in a template of a master workflow loses RPA so you need to create a new association in this case.

Notes and **warnings**:

1. The real validity of a used robot permission will be emerged at submission process, when you run your workflow (not valid robot permission will caused an error in submission). In workflow configuration process you just know that your robot permission data is on the **MyProxy** or not.

2. To use robot certification for job submission by **direct cloud solution**, you need to do some important preliminary tasks:

- Configure your corresponding job(s) with robot certificate by adding robot permission association (about robot permission creation see chapter 20).

- Copy the content of directory *apache-tomcat-6.0.37/temp/dci_bridge/robotcert* to the same directory of the image that contains the slave DCI Bridge (see description of *task 1* at the beginning of this chapter). About image preparation and downloading see *chapter VI* within *Admin Manual*.

- Submit your workflow.

See details about workflow submission by direct cloud solution at *chapter 18* within *Menu-Oriented Online Help*.

3. You can't add robot permission association in case of applying **remote executable**. (For more details about defining remote executable see chapter 14.)

About the robot permission related logging of job submissions and about the user role adding/removing please, see the section *Additional Enhancements* in the *Administrator Manual*.

21. Data Avenue

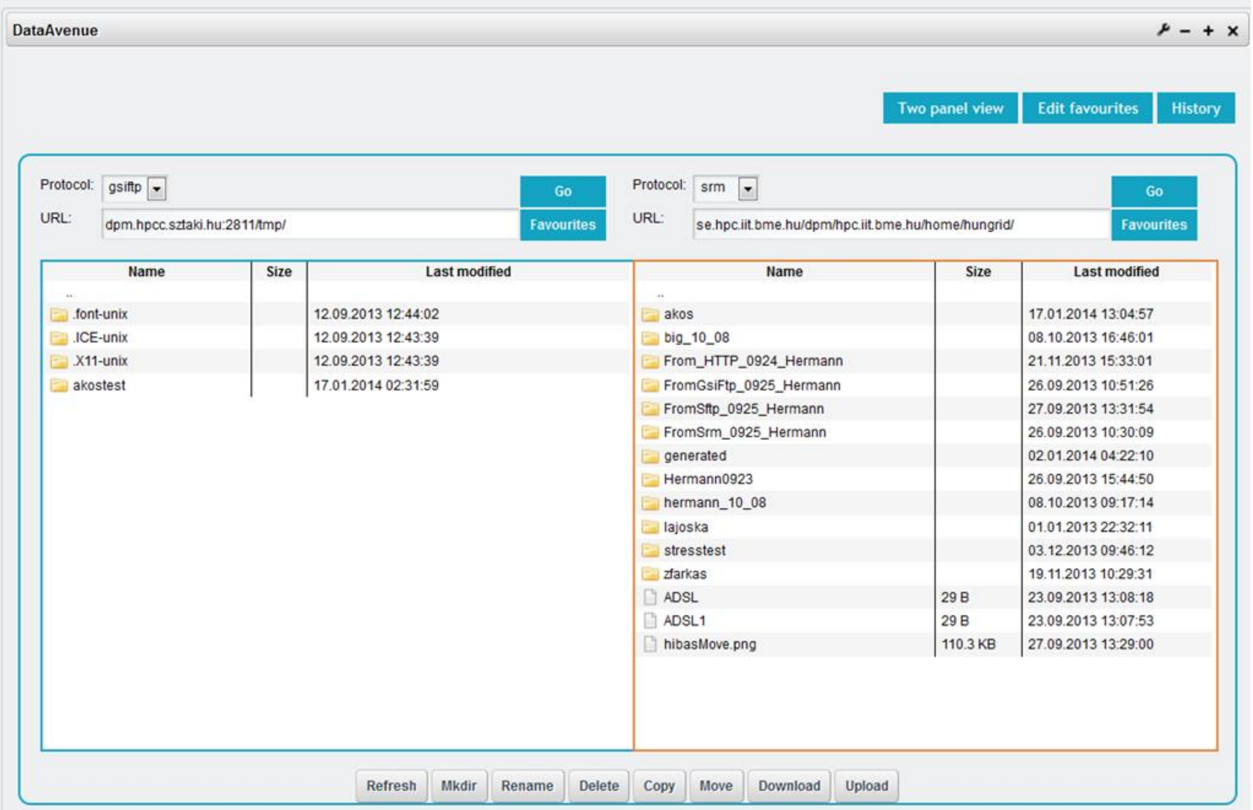
The **Data Avenue** is a file commander tool for data transfer, enabling easy data moving between various storage services (such as grid, cloud, cluster, supercomputers) by various protocols: **HTTP, HTTPS, SFTP, GSIFTP, S3** and **SRM**). The Data Avenue is integrated into WS-PGRADE as a portlet.

With Data Avenue you can up- and download your data to storage services for scientific computation. Additionally, you can copy, move and delete files as well as you can create and copy folders.

The Data Avenue capabilities:

- Convenient, user-friendly solution to connect storages instead of command-line.
- Widespread support of protocols, enabling data moving between various distributed computing infrastructure (DCI) resource storages by various transfer protocols.
- Asynchronous file transfer.
- Data transfer without using of local environment for temporarily storing files.

Warning: The *space* character is not supported in file names. Therefore, you can't use any available operations for a file which has space(s) in their name.



Protocol: gsiftp
URL: dpm.hpcc.sztaki.hu:2811/tmp/

Name	Size	Last modified
..		
.font-unix		12.09.2013 12:44:02
.ICE-unix		12.09.2013 12:43:39
.X11-unix		12.09.2013 12:43:39
akostest		17.01.2014 02:31:59

Protocol: srm
URL: se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/

Name	Size	Last modified
..		
akos		17.01.2014 13:04:57
big_10_08		08.10.2013 16:46:01
From_HTTP_0924_Hermann		21.11.2013 15:33:01
FromGsiFtp_0925_Hermann		26.09.2013 10:51:26
FromSftp_0925_Hermann		27.09.2013 13:31:54
FromSrm_0925_Hermann		26.09.2013 10:30:09
generated		02.01.2014 04:22:10
Hermann0923		26.09.2013 15:44:50
hermann_10_08		08.10.2013 09:17:14
lajoska		01.01.2013 22:32:11
stresstest		03.12.2013 09:46:12
zfarkas		19.11.2013 10:29:31
ADSL	29 B	23.09.2013 13:08:18
ADSL1	29 B	23.09.2013 13:07:53
hibasMove.png	110.3 KB	27.09.2013 13:29:00

Appendix Figure 21.1 Data Avenue – *Two Panel view*

In order to use Data Avenue in WS-PGRADE you need to

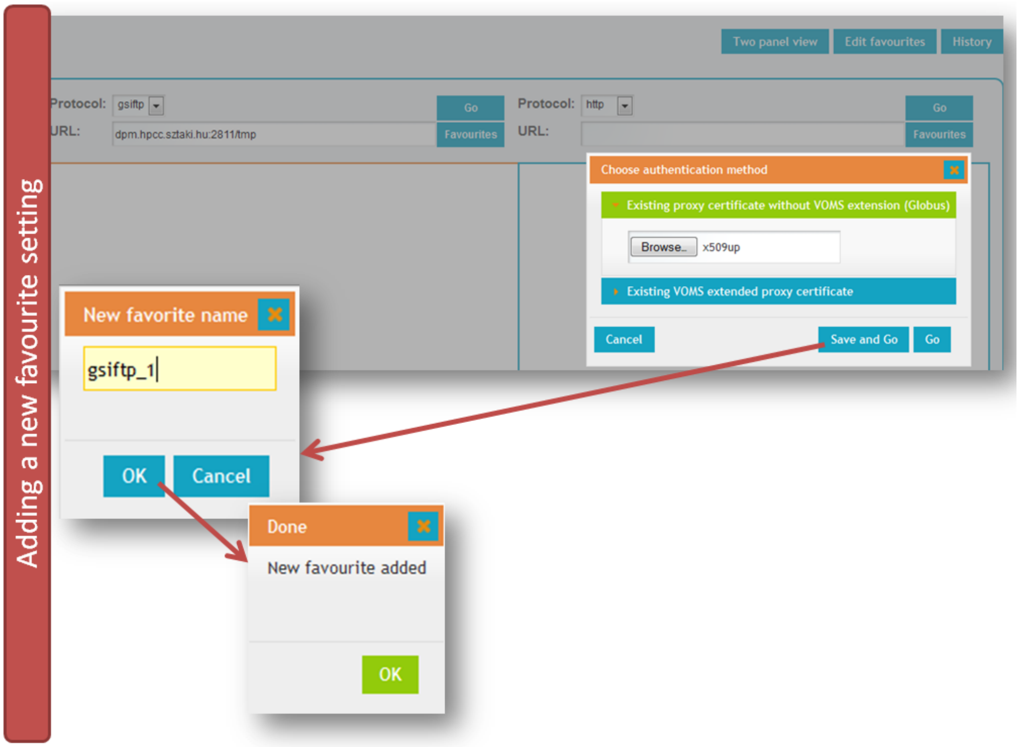
- have a **portal ticket** (to request for a ticket is an administrator's task – see details in chapter *Ticket Requesting to Use Data Avenue* of *Admin Manual*)
- have access to the infrastructures you are planning to use
- own credentials (such as keys, passwords, other authentication data depending on the used protocols) for grids and clouds as well as you have to know the corresponding URLs to access remote data sources.

The use of Data Avenue is very similar to a file commander (like Total Commander or Midnight Commander) with a simple two-panel (source and destination) form for data transfer. (see Appendix Figure 21.1).

A typical scenario for using Data Avenue:

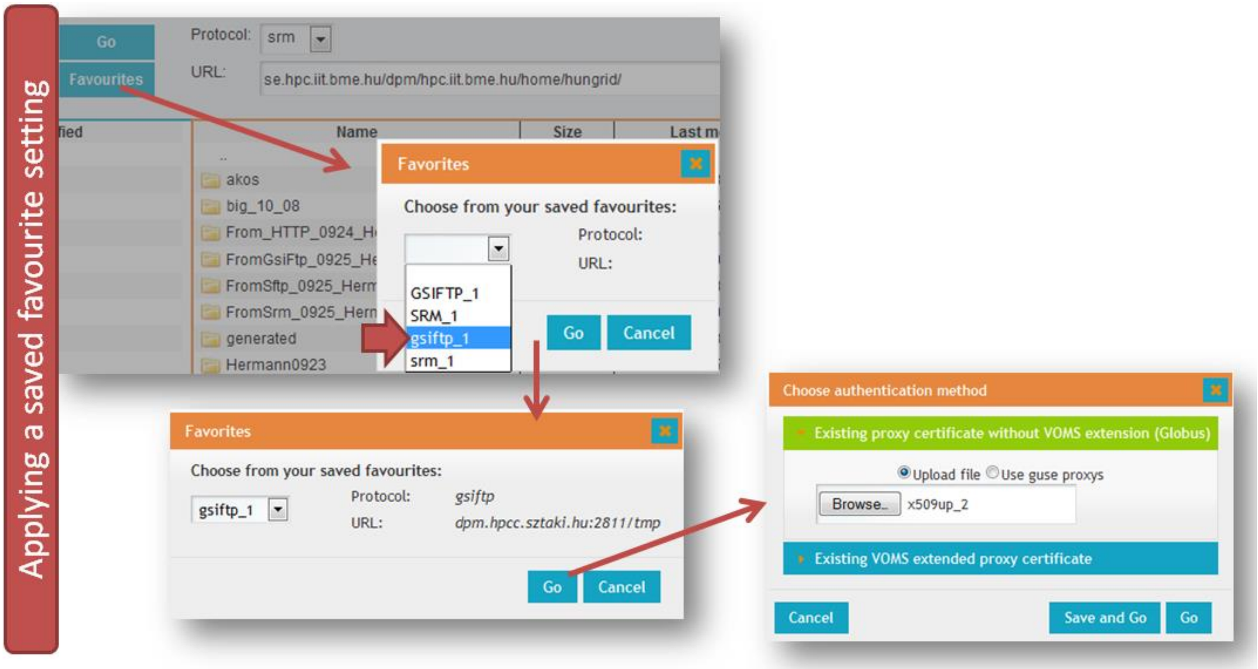
1. Select a *Protocol* from the list box located in the upper left corner.
2. In the next field add *URL* related to the target subdirectory (you can do it from *Favorites* saved earlier – about handling of *Favorites* see Appendix Figure 21.2, 21.3, and 21.4) and then click *Go.*

Notes: The applied authentication method depends on the selected protocol type (see details later). When you apply a saved *Favorite* setting, then you need to use your authentication data again (see Appendix Fig. 21.3)



Protocol: gsiftp
URL: dpm.hpcc.sztaki.hu:2811/tmp
Protocol: http
URL:
Choose authentication method
Existing proxy certificate without VOMS extension (Globus)
x509up
Existing VOMS extended proxy certificate
New favorite name
gsiftp_1
Done
New favourite added

Appendix Figure 21.2 Adding and saving a new favorite setting (resource path, authentication and favorite name)


Applying a saved favourite setting
Go
Favourites
Favorites
Choose from your saved favourites:
Protocol:
URL:
GSIFTP_1
SRM_1
gsiftp_1
srm_1
Go
Cancel
Choose authentication method
Existing proxy certificate without VOMS extension (Globus)
Upload file
Use guse proxys
Browse...
Existing VOMS extended proxy certificate
Save and Go

Protocol: srm

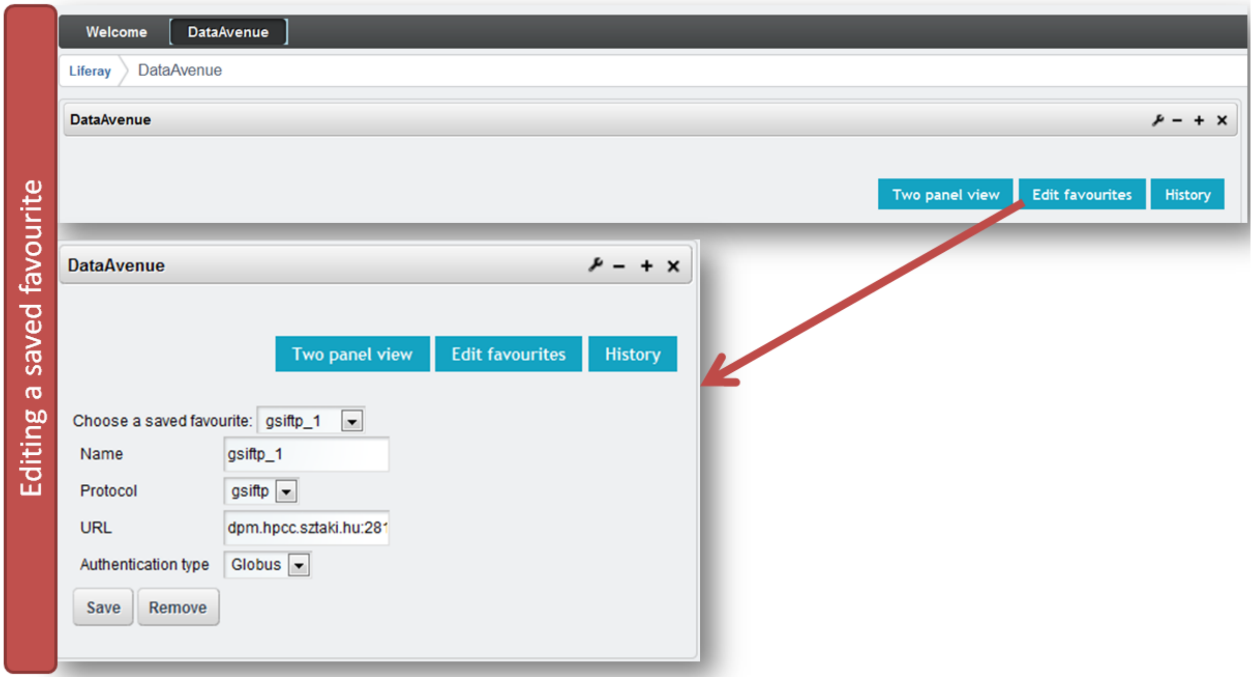
URL: se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/

Choose from your saved favourites: gsiftp_1

Protocol: gsiftp

URL: dpm.hpcc.sztaki.hu:2811/tmp

Appendix Figure 21.3 Applying a favorite setting


Editing a saved favourite
Welcome
DataAvenue
Liferay
DataAvenue
Two panel view
Edit favourites
History
Save
Remove

Choose a saved favourite: gsiftp_1

Name: gsiftp_1

Protocol: gsiftp

URL: dpm.hpcc.sztaki.hu:28

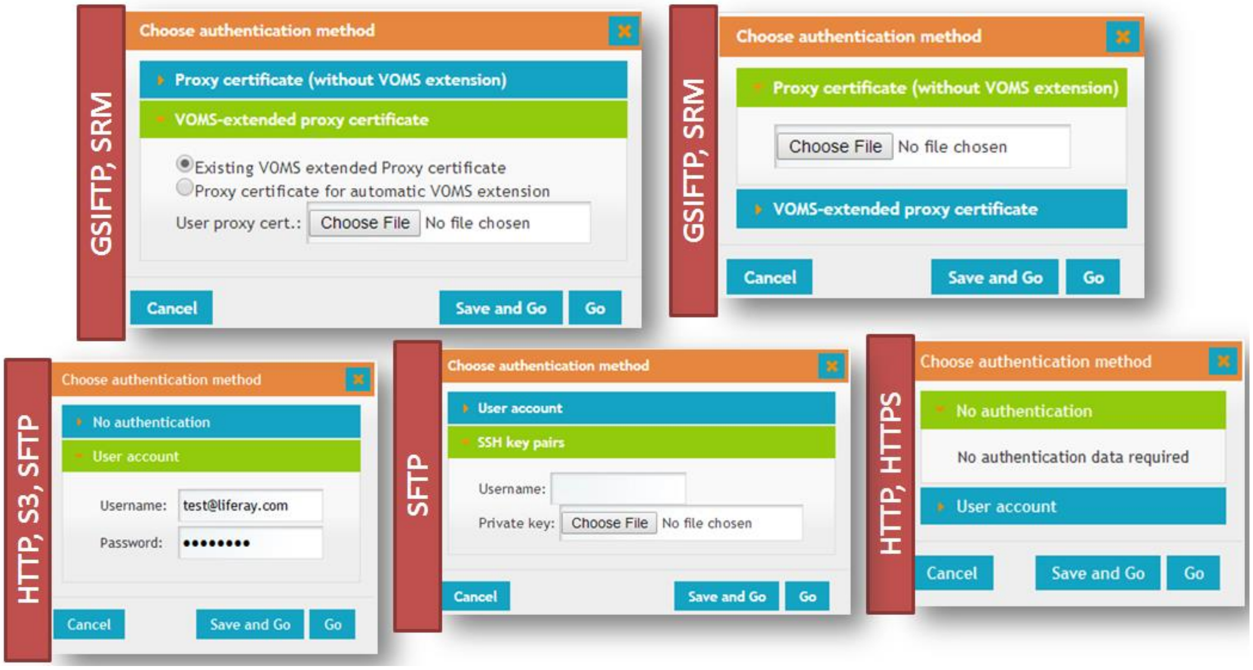
Authentication type: Globus

Appendix Figure 21.4 Editing a *Favorite* properties

3. Add the necessary authentication data in the authentication window. As you read earlier, the applied authentication type depends on the selected protocol. The next table as well as the Appendix Fig. 21.5 show for which protocol which authentication type you need to use.

(Note: In case of S3 protocol you exactly use *access key/secret key* pair intead of username/password)

Protocol	Supported Authentication Types
GSIFTP	[Globus, VOMS]
HTTP	[None, UserPass]
HTTPS	[None]
S3	[UserPass]
SFTP	[UserPass, SSH]
SRM	[Globus, VOMS]


GSIFTP, SRM
Choose authentication method
Proxy certificate (without VOMS extension)
VOMS-extended proxy certificate
User proxy cert.:
Choose File
No file chosen
Cancel
Save and Go
Go
GSIFTP, SRM
Choose authentication method
Proxy certificate (without VOMS extension)
Choose File
No file chosen
VOMS-extended proxy certificate
Cancel
Save and Go
Go
HTTP, S3, SFTP
Choose authentication method
No authentication
User account
Cancel
Save and Go
Go
SFTP
Choose authentication method
User account
SSH key pairs
Username:
Private key:
Choose File
No file chosen
Cancel
Save and Go
Go
HTTP, HTTPS
Choose authentication method
No authentication
User account
Cancel
Save and Go
Go

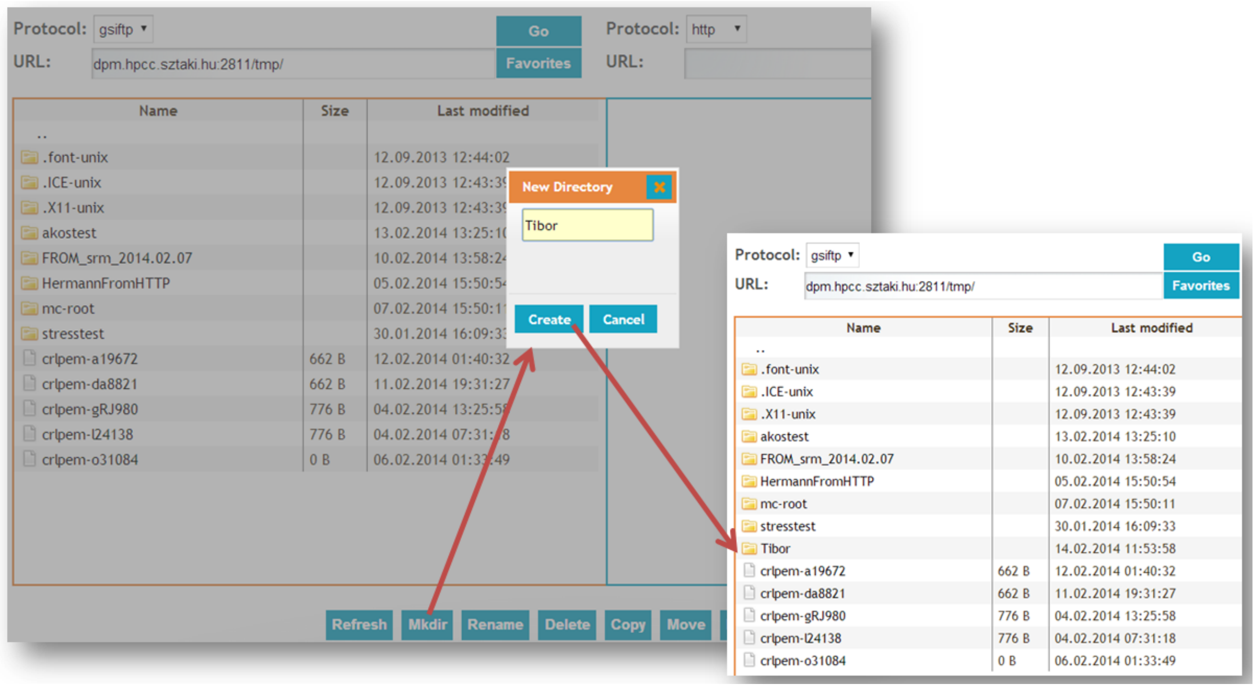
● Existing VOMS extended Proxy certificate
○ Proxy certificate for automatic VOMS extension

Username: test@liferay.com
Password: ••••••••

No authentication data required

Appendix Figure 21.5 Authentication types and protocols

4. At this point you can use the one-panel operations: you can **create**, **delete**, or **rename** your directories, as well as you can **upload/download/refresh** your files.
5. If you want to use a two-panel operation (**copy** or **move**), then you need to perform the steps 1-3 in the second panel as well. Then you need to choose the source and destination panels for operation.
6. Now you can use all available operations.



Protocol: gsiftp
URL: dpm.hpcc.sztaki.hu:2811/tmp/

Protocol: http
URL:

Tibor

Protocol: gsiftp
URL: dpm.hpcc.sztaki.hu:2811/tmp/

Name	Size	Last modified
..		
.font-unix		12.09.2013 12:44:02
.ICE-unix		12.09.2013 12:43:39
.X11-unix		12.09.2013 12:43:39
akostest		13.02.2014 13:25:10
FROM_srm_2014.02.07		10.02.2014 13:58:24
HermannFromHTTP		05.02.2014 15:50:54
mc-root		07.02.2014 15:50:11
stresstest		30.01.2014 16:09:33
Tibor		14.02.2014 11:53:58
crlpem-a19672	662 B	12.02.2014 01:40:32
crlpem-da8821	662 B	11.02.2014 19:31:27
crlpem-gRJ980	776 B	04.02.2014 13:25:58
crlpem-l24138	776 B	04.02.2014 07:31:18
crlpem-o31084	0 B	06.02.2014 01:33:49

Appendix Figure 21.6 A one-panel operation: *Mkdir* (directory creation)

These are the 8 supported operations in Data Avenue (You can find the operation buttons down in the middle):

One-panel operations:

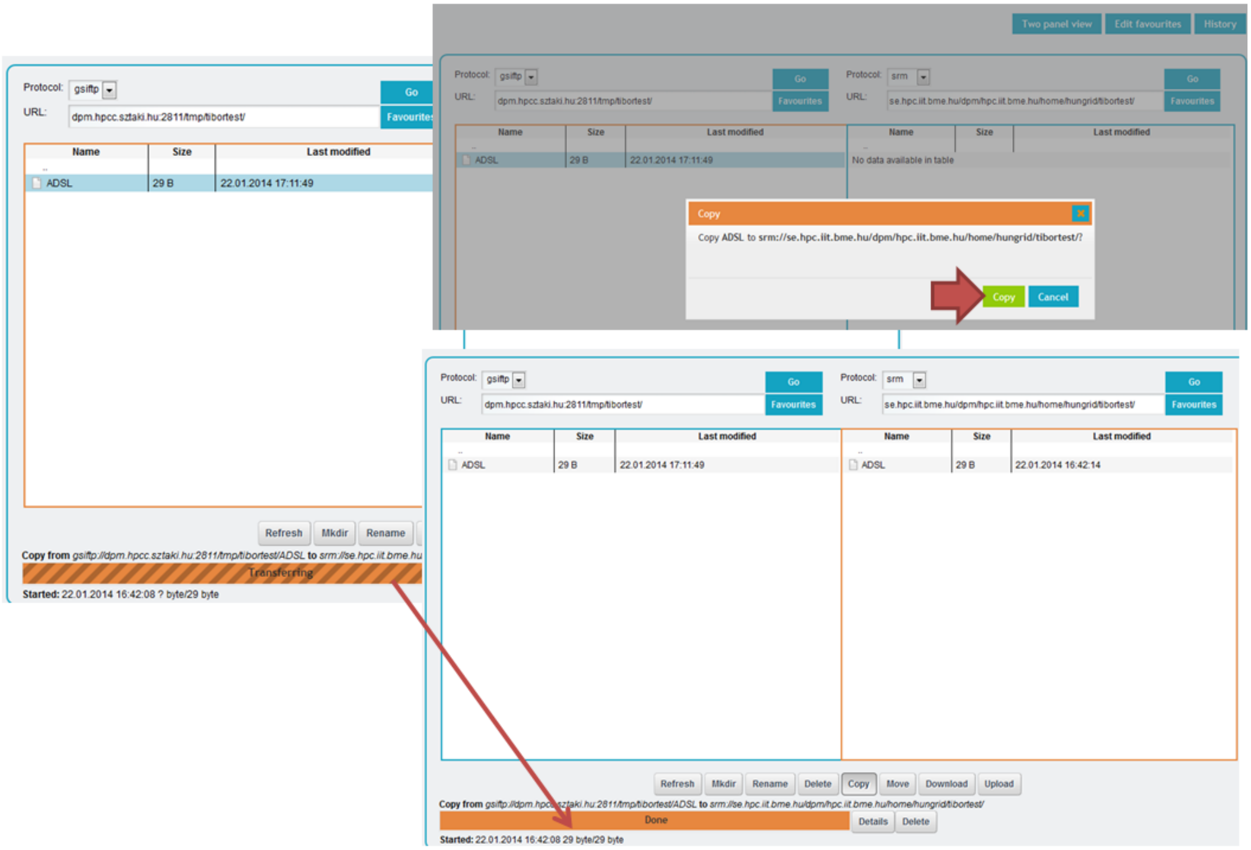
- *Refresh* (current directory contents)
- *Mkdir* (new subdirectory in the current directory; a sample *Copy* operation is shown by Appendix Fig. 21.6)
- *Rename* (the selected file or directory)
- *Delete* (the selected file or directory)
- *Download* (the selected file to your local hard drive)
- *Upload* (a file from your local hard drive to the current remote directory)

Two-panel operations:

- *Copy* (the selected source file or directory to the destination directory; a sample *Copy* operation is shown by Appendix Fig. 21.7)
- *Move* (the selected source file or directory to the destination directory)

Upload, *copy* and *move* operations are executed asynchronously. These operations may require *Refresh* command to update the directory contents in the corresponding side.

Note: Certainly, in case of HTTP/HTTPS protocols you can't *write* the files, therefore the download/upload operations are enabled.


Two panel view
Edit favourites
History
Go
Favourites
Copy
Cancel
Refresh
Mkdir
Rename
Delete
Copy
Move
Download
Upload
Details
Delete

Protocol: gsiftp

URL: dpm.hpcc.sztaki.hu:2811/tmp/tibortest/

Name	Size	Last modified
..		
ADSL	29 B	22.01.2014 17:11:49

Copy from *gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL* **to** *srm://se.hpc.iit.bme.hu*

Transferring

Started: 22.01.2014 16:42:08 ? byte/29 byte

Protocol: srm

URL: se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/

Name	Size	Last modified
..		
No data available in table		

Copy

Copy ADSL to srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/?

Name	Size	Last modified
..		
ADSL	29 B	22.01.2014 16:42:14

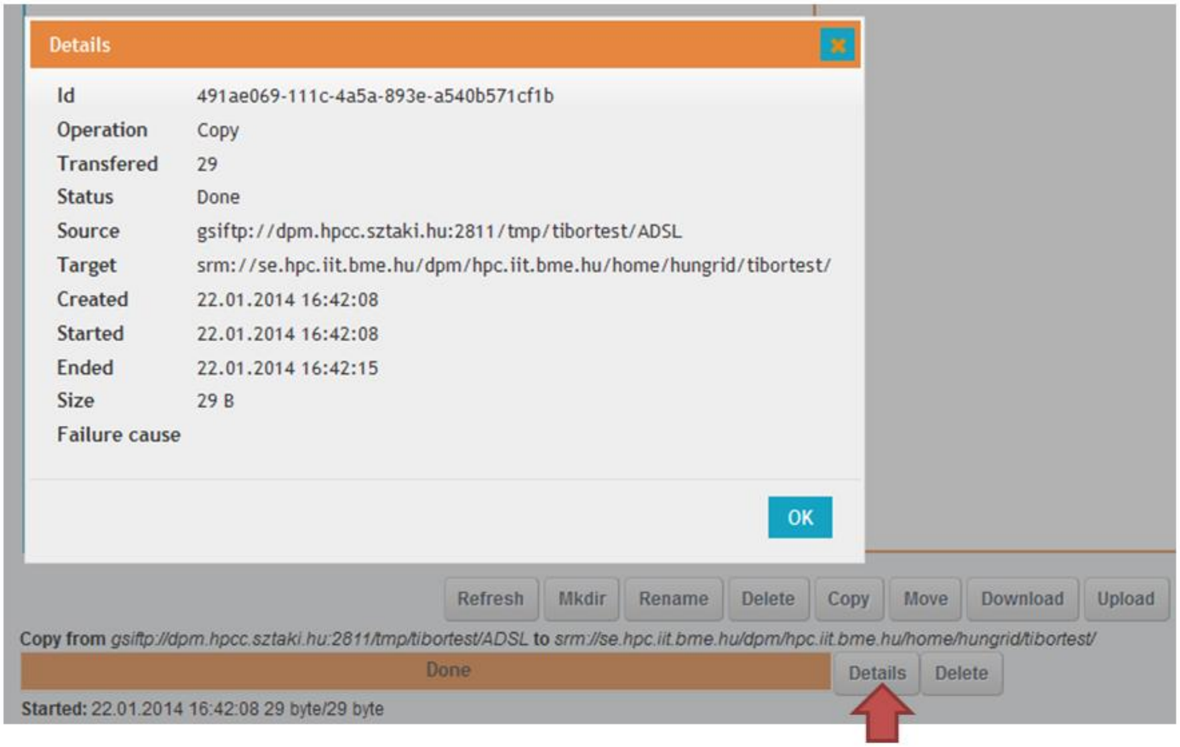
Copy from *gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL* **to** *srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/*

Done

Started: 22.01.2014 16:42:08 29 byte/29 byte

Appendix Figure 21.7 A two-panel operation: *Copy*

You can also use the *Details* and the *History* functions to review the details of the currently and earlier performed operations in Data Avenue (see Appendix Fig. 21.8 and 21.9).


Details
OK
Refresh
Mkdir
Rename
Delete
Copy
Move
Download
Upload
Details
Delete

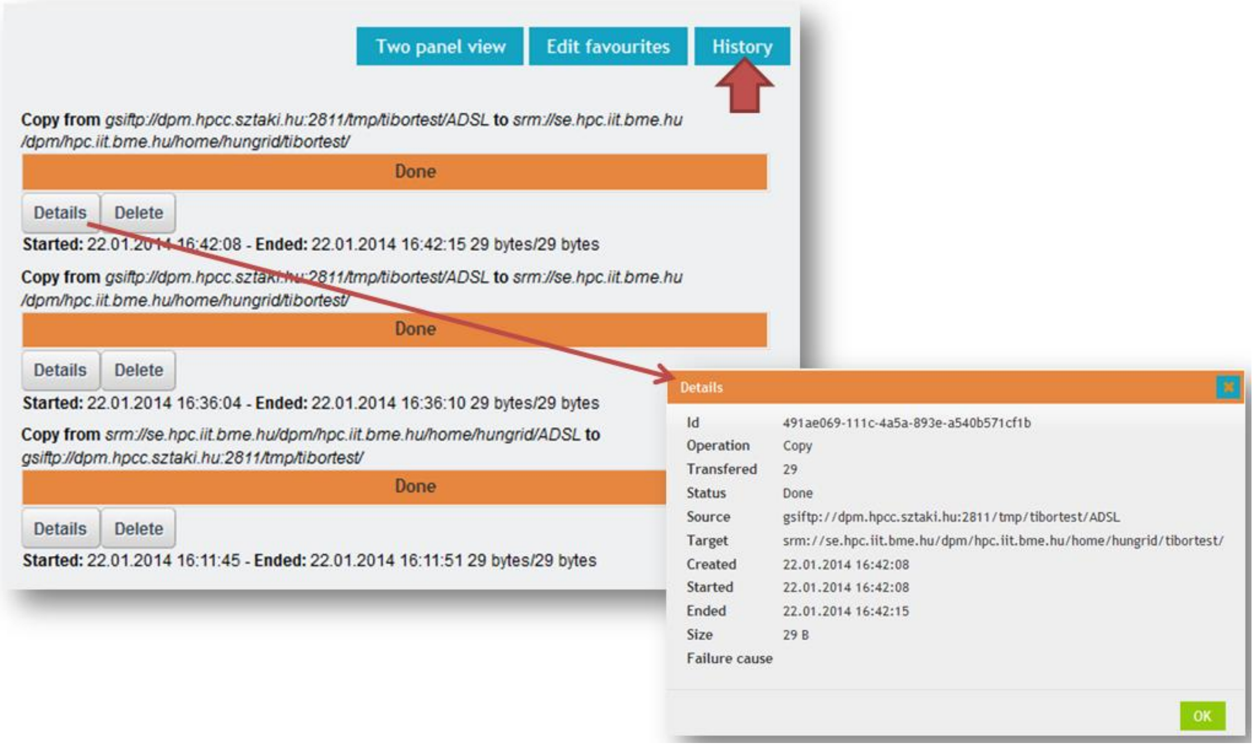
Id 491ae069-111c-4a5a-893e-a540b571cf1b
Operation Copy
Transfered 29
Status Done
Source gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL
Target srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/
Created 22.01.2014 16:42:08
Started 22.01.2014 16:42:08
Ended 22.01.2014 16:42:15
Size 29 B
Failure cause

Copy from *gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL* **to** *srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/*

Done

Started: 22.01.2014 16:42:08 29 byte/29 byte

Appendix Figure 21.8 A *Details* function after a completed Copy operation


Two panel view
Edit favourites
History
Details
Delete
Details
Delete
Details
Delete
Details
OK

Copy from *gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL* **to** *srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/*

Done

Started: 22.01.2014 16:42:08 - **Ended:** 22.01.2014 16:42:15 29 bytes/29 bytes

Copy from *gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL* **to** *srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/*

Done

Started: 22.01.2014 16:36:04 - **Ended:** 22.01.2014 16:36:10 29 bytes/29 bytes

Copy from *srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/ADSL* **to** *gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/*

Done

Started: 22.01.2014 16:11:45 - **Ended:** 22.01.2014 16:11:51 29 bytes/29 bytes

Id 491ae069-111c-4a5a-893e-a540b571cf1b
Operation Copy
Transfered 29
Status Done
Source gsiftp://dpm.hpcc.sztaki.hu:2811/tmp/tibortest/ADSL
Target srm://se.hpc.iit.bme.hu/dpm/hpc.iit.bme.hu/home/hungrid/tibortest/
Created 22.01.2014 16:42:08
Started 22.01.2014 16:42:08
Ended 22.01.2014 16:42:15
Size 29 B
Failure cause

Appendix Figure 21.9 The *History* function

22. Desktop Grid Access from WS-PGRADE

The Desktop Grid (DG) access is solved in gUSE/WS-PGRADE. You can use DG resource to submit your jobs from WS-PGRADE by two ways.

1. You can use the **BOINC (Berkeley Open Infrastructure for Network Computing)** as DG resource. The BOINC technology means a special way of application solving, where the given application have a (single) master (many) slave structure. A BOINC server stores the slave executables of the predefined applications. The slave executables may run on any of the client machines have been subscribed for the given application. The set of associated clients of a given BOINC server compose a BOINC Community. These communities can be regarded as grids, and they have a grid ID within a given BOINC Server. As the **3G Bridge** (see 3G Bridge manual here: http://doc.desktopgrid.hu/doku.php?id=component:3gbridge) is a generic back end component of gUSE system it may host one or more BOINC servers. In order to use a given BOINC project's 3G Bridge service, a 3G Bridge WSDL file has to be prepared that contains access information for the *WSSubmitter* service of the selected 3G Bridge service. (see details in chapter 2.9 within DCI Bridge Manual). A workflow job can be configured to select as BOINC job one of the listed executables codes whose state is true. (See Part D of Appendix Figure 13.)

2. You can use the **GBAC (Generic BOINC Application Client)** -based submission solution. GBAC is a virtualization enabled **wrapper** application. GBAC also represents a generic framework providing virtualized environments for various distributed computing infrastructures (DCIs).
   GBAC is a special variation of the BOINC technology. In the original BOINC the jobs to be executed must have a preinstalled executable on the BOINC server. In case of GBAC this executable will be replaced by a preinstalled computer image file. This image is able to execute the run time received job executable. Therefore slave machines of the BOINC community which are able to receive GBAC jobs must have a virtual execution enabled instruction set and must contain the Virtual Box application. The user can define an own executable - and not only one from a predefined list as in case of BOINC - in order to execute a code on a donated client machine of the selected Desktop Grid community. (See the Workflow/Job Configuration: see Part E of Appendix Figure 13.)

Note: If the job code executed on GBAC-based resource, the name extension for internal output prefix (where 0 <= index < n, and n is the number of generated generator output port files) is not happened. Therefore, it is not recommended to run a generator-type job on GBAC resource.

About BOINC and GBAC plugin settings please, see chapter 2.9 and 2.13 in DCI Bridge Manual.

About the necessary administrative tasks you find description in Admin Manual.

23. SHIWA Submission Service Usage in WS-PGRADE

23.1 Introduction

WS-PGRADE enables you to use the so-called **SHIWA (SHaring Interoperable Workflows for large-scale scientific simulations on Available DCIs)**[8] **Submission Service** for job submission.

The web service based SHIWA Submission Service replaced the old GT4-based GEMLCA Service enabling execution of workflows based on different workflow engines. The common fundamental feature of the old and the new (SHIWA Submission Service and GEMLCA Service) submission services is to enable the deployment of legacy executable code applications as workflows by avoiding the re-engineering of legacy code or by avoiding the access the source files.

However, having SHIWA Submission Service, you can execute non-native workflows in a more reliable and secure way than with the GEMLCA Service. Therefore, you can access workflows remotely from WS-PGRADE and you can submit them from the WS-PGRADE by the help of SHIWA Submission Service.

The essential advantage of SHIWA Submission Service is that you can use various workflows from various communities developed in various engines. All of these workflows are stored in the central workflow repository (called **SHIWA Workflow Repository**).

23.2 Workflow Selection and Configuration

If you want to configure and submit workflow by the SHIWA Submission Service you need to do the followings:

1. First, you need to decide which SHIWA-workflow (stored in the SHIWA Workflow Repository) you want to submit (the legacy executables storing in the SHIWA Workflow Repository are referenced in WS-PGRADE as **Submittable Execution Nodes - SENs**). You can online browse SHIWA-workflows in the central SHIWA Workflow Repository[9] web site (http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/)

Note: you find more information about SHIWA Workflow Repository here: http://repo-test.cpc.wmin.ac.uk/shiwa-repo/resources/user_manual.pdf)

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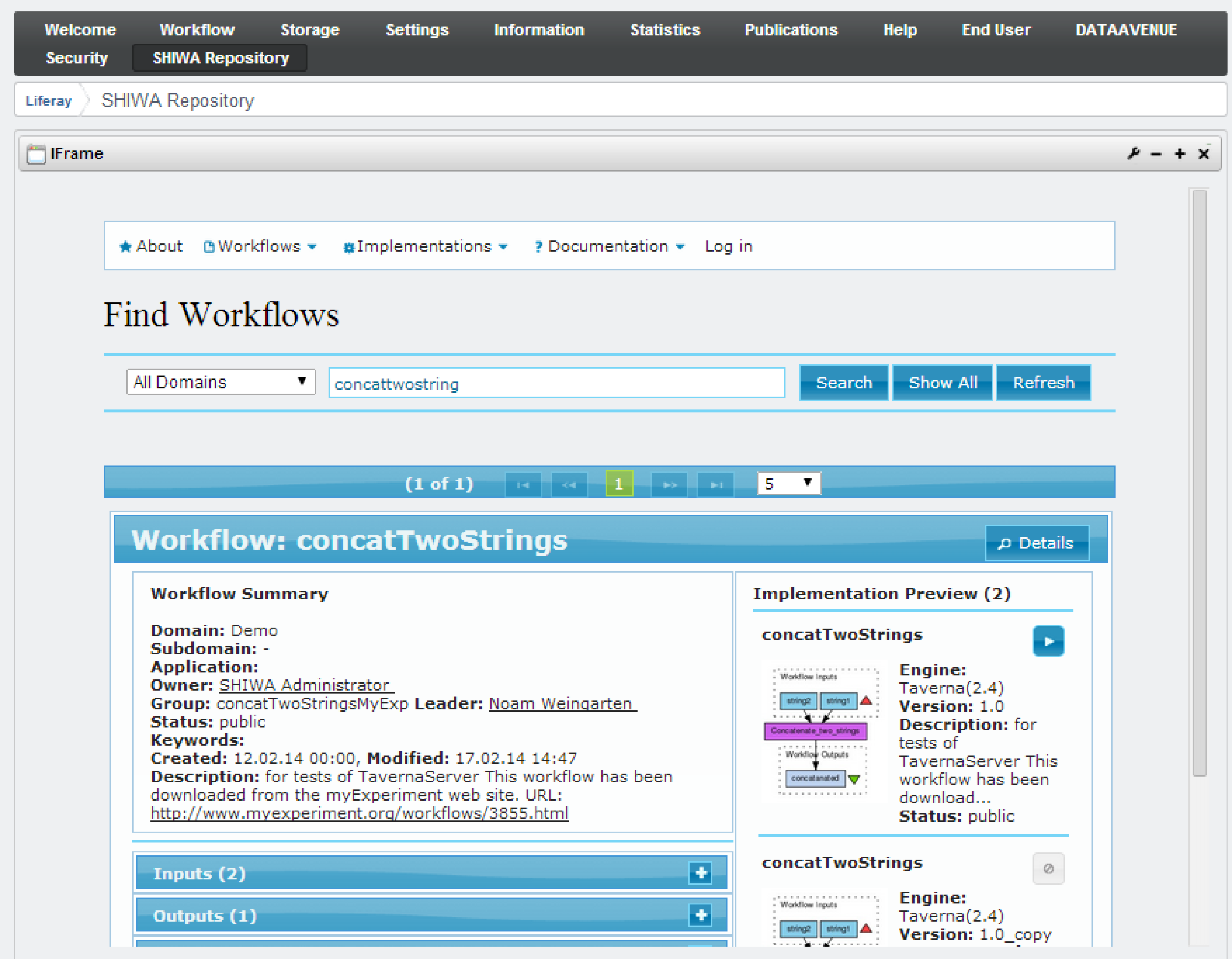
[8] The SHIWA name comes from the FP7 SHIWA project that addresses the challenges of the coarse- and fine-grained workflow interoperability. The project created the SHIWA Simulation Platform which enables users to create and run embedded workflows which incorporate workflows of different workflow systems. The platform consists of the SHIWA Science Gateway and the SHIWA VO.

[9] The SHIWA Workflow Repository manages workflow descriptions, and implementations and configurations of workflows. The repository can be used by the following types of actors:

- E-scientists: They can browse and search the repository to find and download workflows. They can use the repository without registration.
- Workflow developers: They are the workflow owners who can upload, modify and delete workflows. They should register with the repository.
- Repository administrator: The actor who manages the repository.

Otherwise, you can embed into your WS-PGRADE portal the SHIWA Workflow Repository site (see Appendix Fig. 23.1). The necessary administrative Liferay-based configuration details of embedding you find in chapter VIII of Admin Manual.


Welcome
Workflow
Storage
Settings
Information
Statistics
Publications
Help
End User
DATAAVENUE
Security
SHIWA Repository
Liferay
SHIWA Repository
IFrame
About
Workflows
Implementations
Documentation
Log in
Find Workflows
All Domains
concattwostring
Search
Show All
Refresh
(1 of 1)
1
5
Details
Workflow Inputs
string2
string1
Concatenate_two_strings
Workflow Outputs
concatenated
Inputs (2)
Outputs (1)

Workflow: concatTwoStrings

Workflow Summary

Domain: Demo
Subdomain: -
Application:
Owner: SHIWA Administrator
Group: concatTwoStringsMyExp **Leader:** Noam Weingarten
Status: public
Keywords:
Created: 12.02.14 00:00, **Modified:** 17.02.14 14:47
Description: for tests of TavernaServer This workflow has been downloaded from the myExperiment web site. URL: http://www.myexperiment.org/workflows/3855.html

Implementation Preview (2)

concatTwoStrings

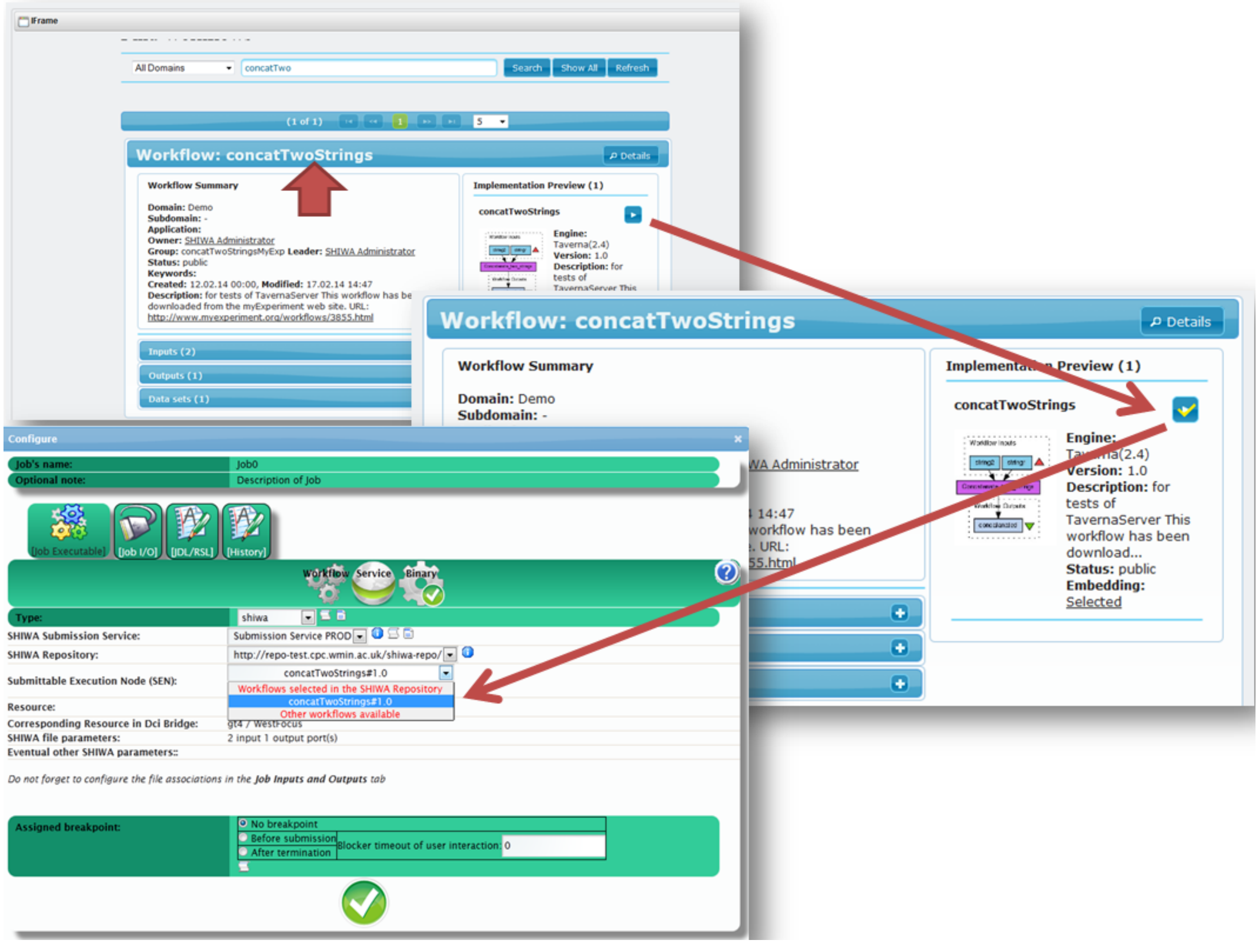
Engine: Taverna(2.4)
Version: 1.0
Description: for tests of TavernaServer This workflow has been download...
Status: public

concatTwoStrings

Engine: Taverna(2.4)
Version: 1.0_copy

Appendix Figure 23.1 Embedded SHIWA Repository web site in the WS-PGRADE

To make the selection of the workflow, you have to click on the *blue arrow button* in the right side. The result of this selection is that your selected workflow will be announced in the *Job Executable* tab, in front of the *Submittable Execution Node (SEN)* list, directly after the *Workflows selected in the SHIWA Repository* label (see Appendix Fig. 23.2)



Workflow: concatTwoStrings

Workflow Summary

Domain: Demo
Subdomain: -
Application:
Owner: SHIWA Administrator
Group: concatTwoStringsMyExp **Leader:** SHIWA Administrator
Status: public
Keywords:
Created: 12.02.14 00:00, **Modified:** 17.02.14 14:47
Description: for tests of TavernaServer This workflow has be… downloaded from the myExperiment web site. URL: http://www.myexperiment.org/workflows/3855.html

Implementation Preview (1)

concatTwoStrings

Engine: Taverna(2.4)
Version: 1.0
Description: for tests of TavernaServer This workflow has been download...
Status: public
Embedding:
Selected

Job's name:	Job0
Optional note:	Description of Job
Type:	shiwa
SHIWA Submission Service:	Submission Service PROD
SHIWA Repository:	http://repo-test.cpc.wmin.ac.uk/shiwa-repo/
Submittable Execution Node (SEN):	concatTwoStrings#1.0 Workflows selected in the SHIWA Repository concatTwoStrings#1.0 Other workflows available
Resource:	
Corresponding Resource in Dci Bridge:	gt4 / WestFocus
SHIWA file parameters:	2 input 1 output port(s)
Eventual other SHIWA parameters::	

*Do not forget to configure the file associations in the **Job Inputs and Outputs** tab*

Assigned breakpoint:
● No breakpoint
○ Before submission
○ After termination
Blocker timeout of user interaction: 0

Appendix Figure 23.2 A SHIWA-workflow selection in the SHIWA Repository portlet

If you decide which SEN you want to submit, then you can go to the WS-PGRADE runtime look up system, **SHIWA Explorer** (in the *Information/SHIWA Explorer* menu – more details in chapter 8). Here you can find your desired SEN together with the related file parameters. Within a selected SHIWA Submission Service and SHIWA Repository the available SENs are listed in the SHIWA Explorer. Among the listed SENs you can search for your earlier saw one in the SHIWA Workflow Repository web site. Once you found it and selected it in the SHIWA Explorer, you get the listed parameters description of SEN (see Appendix Fig. 23.3). This information will be useful in the workflow creation and configuration phase (step 4).

Summarizing the possibilities of workflow (SEN) selection, you can use four methods for looking up workflows:

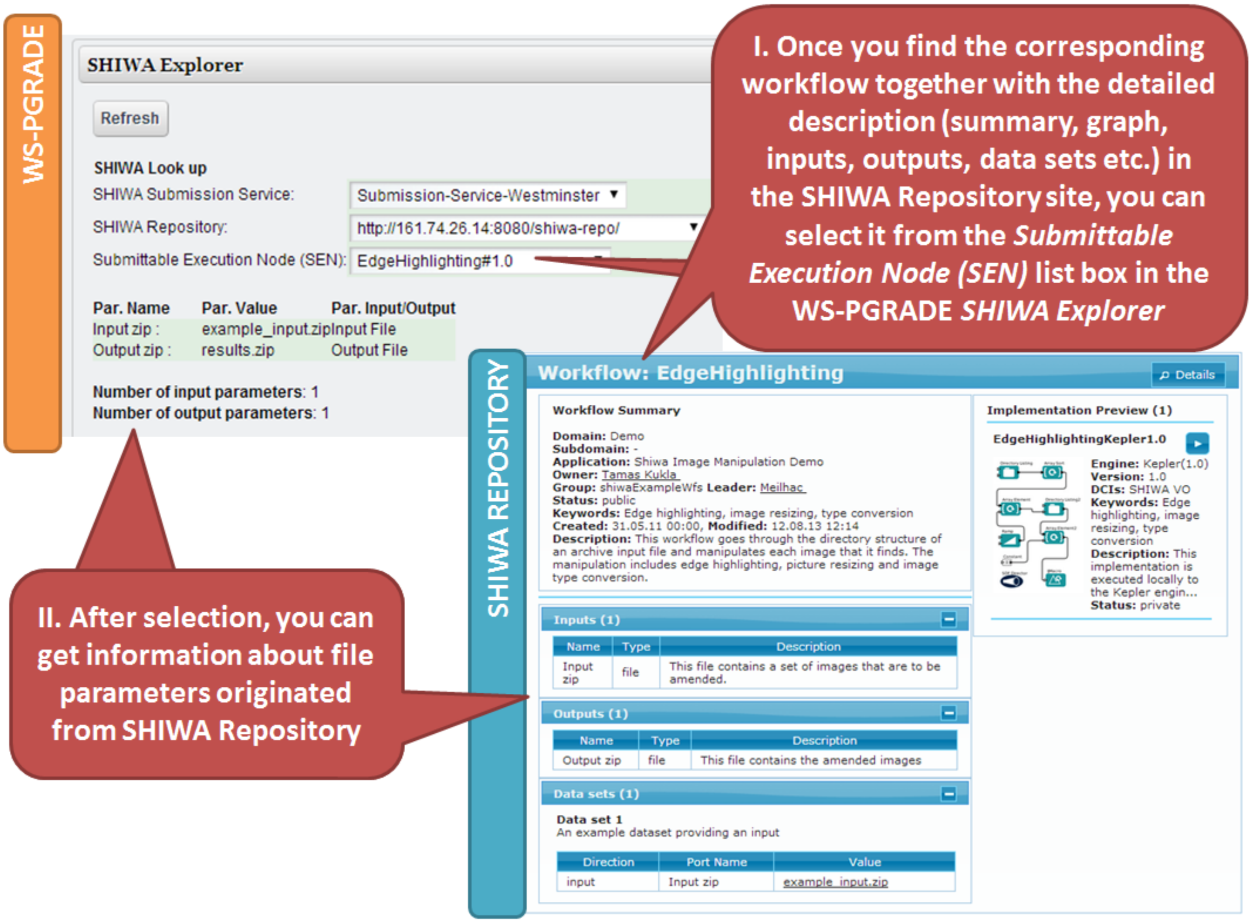
a. You can access the SHIWA Workflow Repository web site by a web browser.
b. You can access the SHIWA Workflow Repository web site content directly from a WS-PGRADE portal.

c. You can use *SHIWA Explorer* for a simple workflow browsing within WS-PGRADE.
d. You have to use the *Submittable Execution Node (SEN)* list box within the *Job Executable* tab to select a workflow (SEN) for configuration.

Option *a.* and *b.* are good for an easy and convenient preselection of workflows; option b. is also usable to add the selected workflow to the first rows in the SEN list within option *d*; option *d*. is mandatory (there is a step of configuration – see step 3).

2. Now you know the details of the workflow you want to submit. Therefore you can create it in the *Graph Editor*. (As you see in the example of Appendix Fig. 23.3 the selected SEN has one input parameter and one output parameter – thus, the created node has to be one input and one output parameter too.)

Note: In the created workflow the number of input file parameters must correspond to the number of input ports of the enveloping job from SHIWA Repository and the number of the output file parameters must correspond to the number of the output ports of the enveloping job of SHIWA Repository.



I. Once you find the corresponding workflow together with the detailed description (summary, graph, inputs, outputs, data sets etc.) in the SHIWA Repository site, you can select it from the ***Submittable Execution Node (SEN)*** list box in the WS-PGRADE ***SHIWA Explorer***

II. After selection, you can get information about file parameters originated from SHIWA Repository

SHIWA Explorer

SHIWA Look up

SHIWA Submission Service: Submission-Service-Westminster
SHIWA Repository: http://161.74.26.14:8080/shiwa-repo/
Submittable Execution Node (SEN): EdgeHighlighting#1.0

Par. Name	Par. Value	Par. Input/Output
Input zip :	example_input.zip	Input File
Output zip :	results.zip	Output File

Number of input parameters: 1
Number of output parameters: 1

Workflow: EdgeHighlighting

Workflow Summary

Domain: Demo
Subdomain: -
Application: Shiwa Image Manipulation Demo
Owner: Tamas Kukla
Group: shiwaExampleWfs **Leader:** Meilhac
Status: public
Keywords: Edge highlighting, image resizing, type conversion
Created: 31.05.11 00:00, **Modified:** 12.08.13 12:14
Description: This workflow goes through the directory structure of an archive input file and manipulates each image that it finds. The manipulation includes edge highlighting, picture resizing and image type conversion.

Implementation Preview (1)

EdgeHighlightingKepler1.0

Engine: Kepler(1.0)
Version: 1.0
DCIs: SHIWA VO
Keywords: Edge highlighting, image resizing, type conversion
Description: This implementation is executed locally to the Kepler engin...
Status: private

Inputs (1)

Name	Type	Description
Input zip	file	This file contains a set of images that are to be amended.

Outputs (1)

Name	Type	Description
Output zip	file	This file contains the amended images

Data sets (1)

Data set 1
An example dataset providing an input

Direction	Port Name	Value
input	Input zip	example_input.zip

Appendix Figure 23.3 Exploring workflow in WS-PGRADE SHIWA explorer

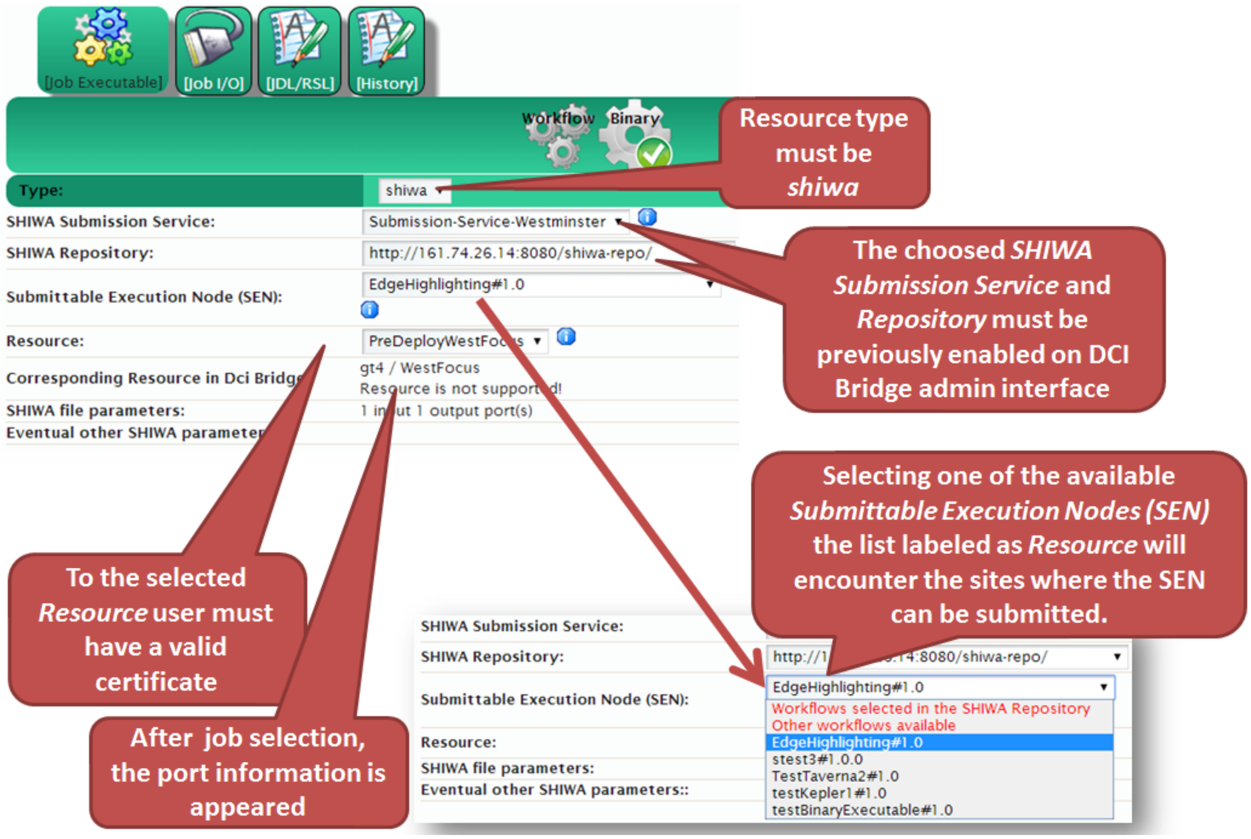
3. Once the graph is ready and saved, then you can configure your workflow. Use the *Workflow/Concrete/Configure* function (see Appendix Fig. 23.3). In this type of configuration you don't need to upload executable for your workflow jobs because these element is available in the SHIWA Workflow Repository. (Additionally, you can also upload your inputs from this site – see next step.)

   The sequence of configuration is as follows in *Job Executable* tab:
   - First, select the necessary *SHIWA Submission Service* and the *SHIWA Repository* from the set of available elements.
   - Then WS-PGRADE will show only those SENs, which fulfill the "interface condition" which you see in SHIWA Explorer: the number of input file parameters must correspond to the number of input ports of the enveloping job and the number of the output file parameters must correspond to the number of the output ports of the enveloping job.
   - By selecting one of the available SENs the next will happen: A form - labeled as *SHIWA file parameters* - will open encountering the list of names and re-definable default values of the – non file like - input parameters of the selected SEN and a list labeled as *Resource* will encounter the sites where proper SEN can be submitted.

Notes:

You can only submit your workflow if you have valid certification for your selected resource. You can check the selected resource in *Job Executable* tab at the *Corresponding Resource in DCI Bridge* property (see Appendix Fig. 23.4 – in the introduced example this resource is the *gt4/WestFocus*).

Don't forget to save your settings by clicking on the check mark in the bottom of *Job Executable* tab.



Type: shiwa

SHIWA Submission Service: Submission-Service-Westminster

SHIWA Repository: http://161.74.26.14:8080/shiwa-repo/

Submittable Execution Node (SEN): EdgeHighlighting#1.0

Resource: PreDeployWestFoc s

Corresponding Resource in Dci Bridg gt4 / WestFocus Resource is not supported!

SHIWA file parameters: 1 input 1 output port(s)

Eventual other SHIWA paramete

Resource type must be *shiwa*

The choosed *SHIWA Submission Service* and *Repository* must be previously enabled on DCI Bridge admin interface

Selecting one of the available *Submittable Execution Nodes (SEN)* the list labeled as *Resource* will encounter the sites where the SEN can be submitted.

To the selected *Resource* user must have a valid certificate

After job selection, the port information is appeared

SHIWA Submission Service:

SHIWA Repository: http://1 :8080/shiwa-repo/

Submittable Execution Node (SEN): EdgeHighlighting#1.0

- Workflows selected in the SHIWA Repository
- Other workflows available
- EdgeHighlighting#1.0
- stest3#1.0.0
- TestTaverna2#1.0
- testKepler1#1.0
- testBinaryExecutable#1.0

Resource:

SHIWA file parameters:

Eventual other SHIWA parameters::

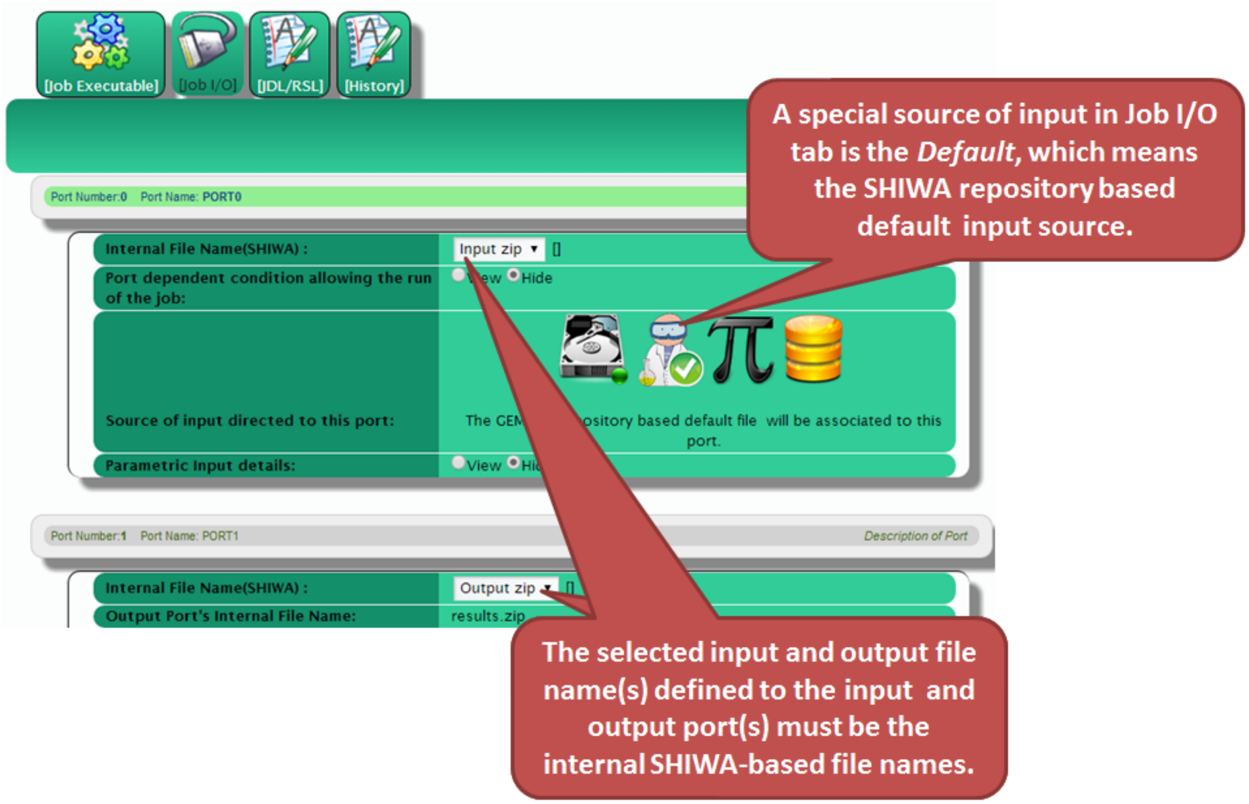
Appendix Figure 23.4 SHIWA-based configuration 1 – Job Executable tab

4. In the *Job I/O* tab you need to choose the corresponding input and output names. Then you can upload by the routine way.

Notes:

A special input source in case of SHIWA-based job I/O settings is the *Default* (the *Default* icon:), which means the **SHIWA repository based default input source** – see Appendix Fig. 23.5) . Thus, among the common methods (uploading, value adding, SQL command using) you can add your input from the remote SHIWA Workflow Repository too.

Don't forget to save your settings by clicking on the check mark in the bottom of *Job I/O* tab.



Port Number:0 Port Name: PORT0

Internal File Name(SHIWA) :	Input zip ▾ []
Port dependent condition allowing the run of the job:	○ ew ● Hide
Source of input directed to this port:	The GEM ository based default file will be associated to this port.
Parametric Input details:	○ View ● Hi

Port Number:1 Port Name: PORT1 *Description of Port*

Internal File Name(SHIWA) :	Output zip ▾ []
Output Port's Internal File Name:	results.zip

A special source of input in Job I/O tab is the *Default*, which means the SHIWA repository based default input source.

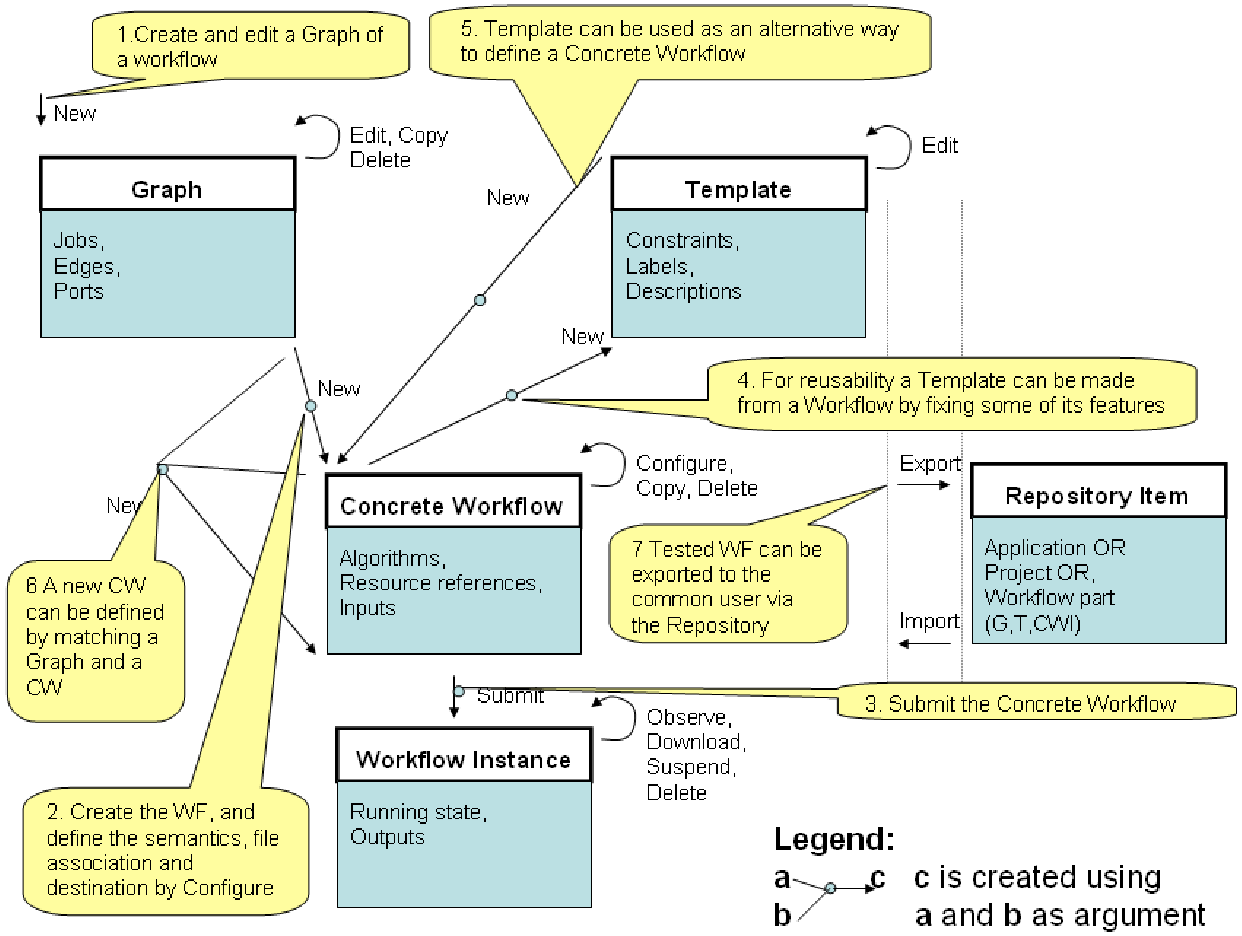
The selected input and output file name(s) defined to the input and output port(s) must be the internal SHIWA-based file names.

Appendix Figure 23.5 SHIWA-based configuration 2 – Job I/O tab

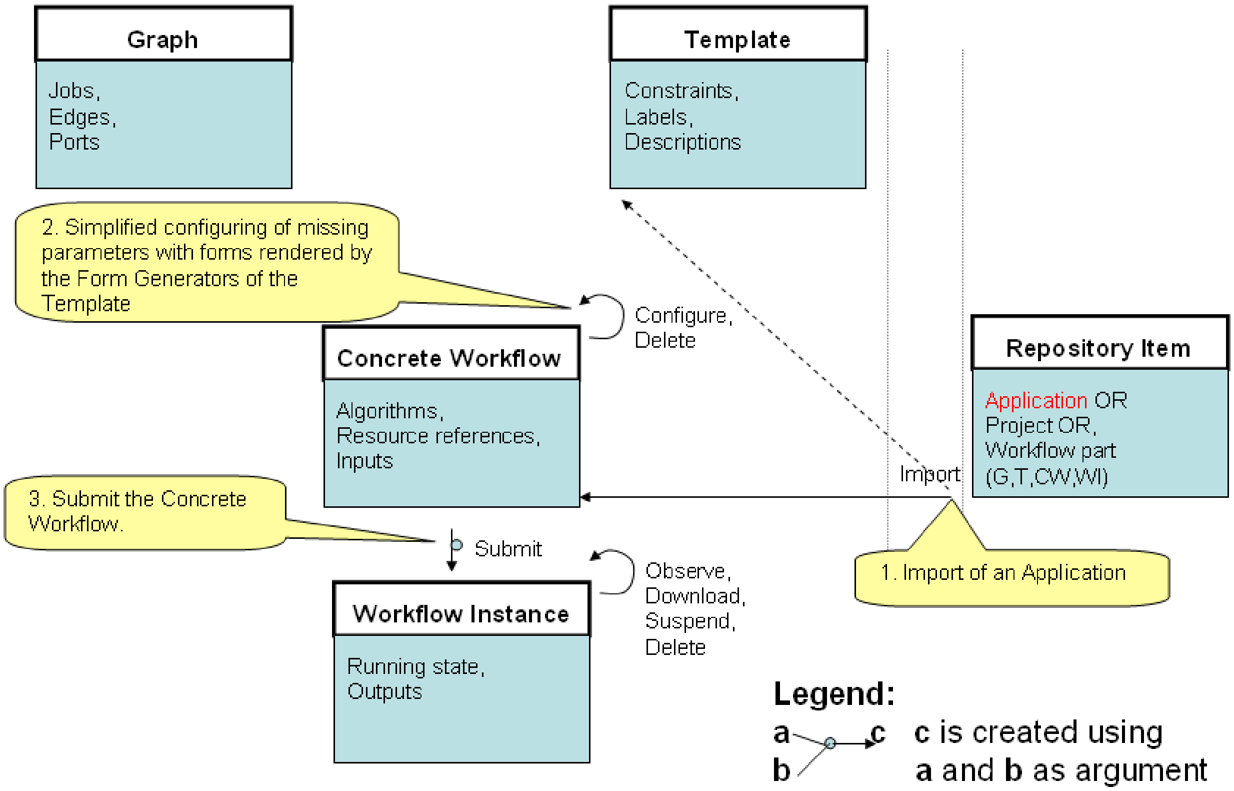
5. Once you configured and saved your workflow, you can submit it by the routine way: clicking on the *Submit* button at the corresponding workflow in the *Workflow/Concrete* window.

Note: You find more details about SHIWA-based job configuration here: http://repo-test.cpc.wmin.ac.uk/shiwa-repo/resources/portal_tutorial.pdf

Main Terms and Activities in the WS-PGRADE Portal (Appendix II)


1.Create and edit a Graph of a workflow
5. Template can be used as an alternative way to define a Concrete Workflow
New
Edit, Copy Delete
Edit
Graph
Jobs, Edges, Ports
New
Template
Constraints, Labels, Descriptions
New
New
4. For reusability a Template can be made from a Workflow by fixing some of its features
New
Configure, Copy, Delete
Export
Concrete Workflow
Algorithms, Resource references, Inputs
Repository Item
Application OR Project OR, Workflow part (G,T,CWI)
6 A new CW can be defined by matching a Graph and a CW
7 Tested WF can be exported to the common user via the Repository
Import
Submit
3. Submit the Concrete Workflow
Observe, Download, Suspend, Delete
Workflow Instance
Running state, Outputs
2. Create the WF, and define the semantics, file association and destination by Configure
Legend:
a
b
c
c is created using a and b as argument

Appendix II Figure 1 Objects created and manipulated by the full power user


Graph
Jobs,
Edges,
Ports
Template
Constraints,
Labels,
Descriptions
2. Simplified configuring of missing parameters with forms rendered by the Form Generators of the Template
Configure,
Delete
Concrete Workflow
Algorithms,
Resource references,
Inputs
Repository Item
Application OR
Project OR,
Workflow part
(G,T,CW,WI)
Import
3. Submit the Concrete Workflow.
Submit
1. Import of an Application
Workflow Instance
Running state,
Outputs
Observe,
Download,
Suspend,
Delete
Legend:
a
b
c
c is created using
a and b as argument

Appendix II Figure 2 Objects created and manipulated by the common user

Jump Start in the Development Cycle (Appendix III)

Introduction

During the following case study a simple example workflow containing a cascade of two jobs (both using the same tested and available binary executable code) will be created, started, and observed. This binary executable reads two input text files named "INPUT1" and "INPUT2" from the working directory of the execution environment as operation arguments. Using these files as the arguments of an integer arithmetic operation (selected by the command line argument "A" for addition, "M" for multiplication, etc.) the program will be executed, and it will produce the result of the operation as an output text file named "OUTPUT", and a verbose listing on the standard output "stdout" and - in case of eventual run time error - on the standard output "stderr". (Appendix Fig. 11)

1. Creating the Graph of the Workflow

In the tab Workflow/Graph the Graph Editor will be started by button "Graph Editor". See Appendix Figure 1

The appearing web start application opens a Graph Editor Window where by the menu commands of groups "Graph" and "Edit" the graph structure (visible on Appendix Figure 2) can be edited and saved.

Appendix Figure 3 shows how the name of a created (menu command Graph/New Job) job can be changed in the Job Properties window.

Right click on the icon of the selected job permits the selection of "Properties", which opens the Job Properties window.

Please note, that a new port appears as an input port; you have to change its properties (selectable by right click) in order to change its Port Type or Port Name (visible in Appendix Figure 4), and only an output port can be connected to a foreign input port (by the described dragging mechanism).

To meet the file name matching convention discussed in the definition of the binary executable (see the Introduction) the port name shown on Appendix Fig. 4 has been chosen as "INPUT1".

The created graph can be saved by the menu command Graph/Save as...

2. Creating the Workflow

The new workflow will be created in the tab Workflow/Create Concrete (see Appendix Figure 5).

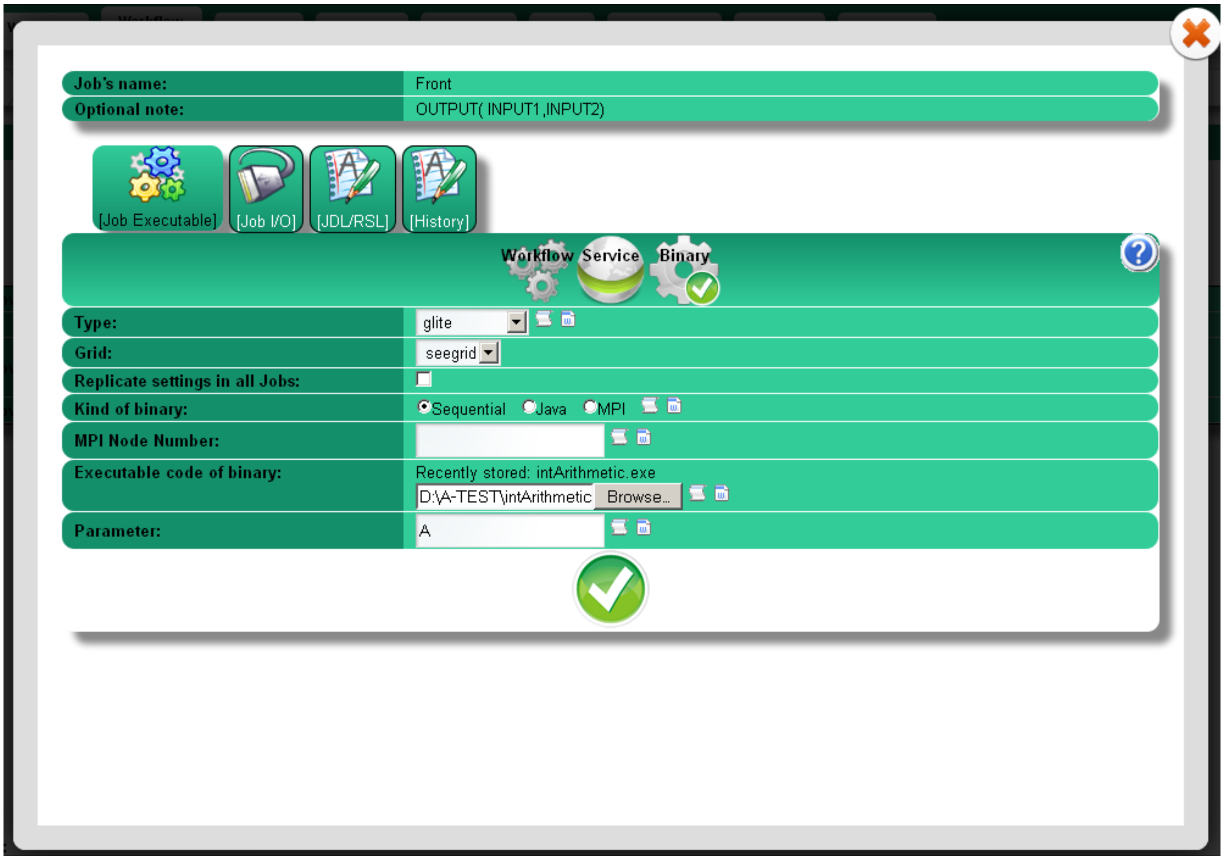
The name of the Graph created in paragraph 1 will be used as frame.

A non-existing new name -in our case "MathOpCascade" - must be defined for the workflow and confirmed by the button "OK".

3. Configuring the Created Workflow

The steps:

1. The configuration must be started by selecting the button "Configure" on the tab Workflow/Concrete in the line belonging to the workflow created in paragraph 2. (See Appendix Figure 6)
2. The frame of the configuration is the window where the job-wise configuration can be started (by clicking on the appropriate job icon) and finally the configuration can be saved on the Portal Server by the appropriate button (See Appendix Figure 12)
3. By selecting a job (discussed in 3.2) a new window appears where the properties of the job can be defined: See the active tab "Job Executable" on the window Appendix Figure 13. Note that the appearance of the actual view may be different from the Figure 13. Please select gLite as Type: in order to get the proper fields! The subsequent window (Appendix III. Figure 1) shows the configuration of a binary code to be send to the VO seegrid by the gLite submitter. Appendix III Figure 1: Job Executable after configuration. The binary code (discussed in the Introduction) will be uploaded from a local archive "D:\A-Test\intArithmetic.exe" and will have the command line parameter "A" which will instruct the code to execute the "addition" operation. The button "Save.." confirms the operation.
4. The port configuration window - by which we will define the file arguments to the required calculation - appears by the direct clicking on the icon of a port of the graph visible in the window mentioned in 3.2 (or by selecting the tab "Job Inputs and Outputs" of the window appearing in 3.3). The Appendix Figure 17 shows the latter case: Each port configuration entry belonging to the current job (in our case job "Front") is enumerated and can be made visible by the slider toward the right side of the window. The Appendix Figure 18 shows, that both input ports of the job "Front" has been associated by the text files which will be uploaded from the selected local archive of the user. The button "OK" (hidden in the Appendix Figure 18 but reachable by moving the mentioned slider) confirms the settings.
5. The state and history of the job configuration can be checked by selecting the tab "Job Configuration History" (See - for example - in Appendix Figure 18). The result will be the listing similar to Appendix Figure 30.
6. The configuration steps 3.3 and 3.4 must be repeated for the job "Tail" including its free input port "1" and terminated by hitting the button "Save on Server" (See Appendix Figure 12)



Job's name:	Front
Optional note:	OUTPUT(INPUT1 ,INPUT2)
Type:	glite
Grid:	seegrid
Replicate settings in all Jobs:	☐
Kind of binary:	● Sequential ○ Java ○ MPI
MPI Node Number:	
Executable code of binary:	Recently stored: intArithmetic.exe D:\A-TEST\intArithmetic
Parameter:	A

Appendix III Figure 1 Job Executable after configuration

4. Obtaining of a Valid Proxy Certificate

The button Download will be hit on tab Certificates (see Figure 15), the proper fields must be filled on the Proxy Download Window (see Figure 17) and subsequently the successfully downloaded proxy certificate must be associated to the resource "seegrid" have been selected in 3.3.

This association can be initialized by the button Set for Grid on the main page of the Certificate manager menu (Figure 15).

5. Checking the Configuration

The error free state of the configuration can be controlled by hitting the button "Info" in the proper line belonging to the workflow in the tab Workflow/Concrete (see Appendix Figure 6).

The result is visible on Appendix Figure 31. (The saved image on Figure 31 shows a case: when the user skipped the "Set for Grid" command in step 4).

6. Submitting the Workflow

The correct workflow can be submitted in the tab Workflow/Concrete by hitting the button "Submit" (see Appendix Figure 6). A user friendly name for the identification of the workflow instance to be created can be defined in the appearing dialogue box.

The main goal of the dialogue box to fit the submission of the workflow, and there is an option to define e-mail notification about the progress/termination of the workflow (see Appendix Figure 7).

7. Controlling the Progress/Termination of the Submitted Workflow

The progress/termination of the submitted workflow instances can be initialized by hitting the button "Details" belonging to the line of the given workflow in the tab Workflow/Concrete (see Appendix Figure 6). The result will be the enumeration of the created workflow instances (see Appendix Figure 8).

7.1 Observing the details of a workflow instance:

Selecting and hitting the button "Details" of a workflow instance (see Appendix Figure 8) the aggregated list of the created job instances of the workflow instance can be reached. The result is visible on Appendix Figure 9.

7.2 Observing the details of Job instances

By selecting the button "View content(s)" belonging to the line of a job (see Appendix Figure 9) the list of job instances will be listed. The result is visible on Appendix Figure 10.

Note, that in case of PS workflows there may be more than 1 instance associated to a given job.

7.3 Access of files belonging to a job instance

A runtime created file associated to given job instance can be reached by hitting the proper buttons belonging to the line of the selected job instance (see Appendix Figure 10).

Appendix Figure 11 shows what the binary executable of job "Tail" writes on the standard output "stdout".

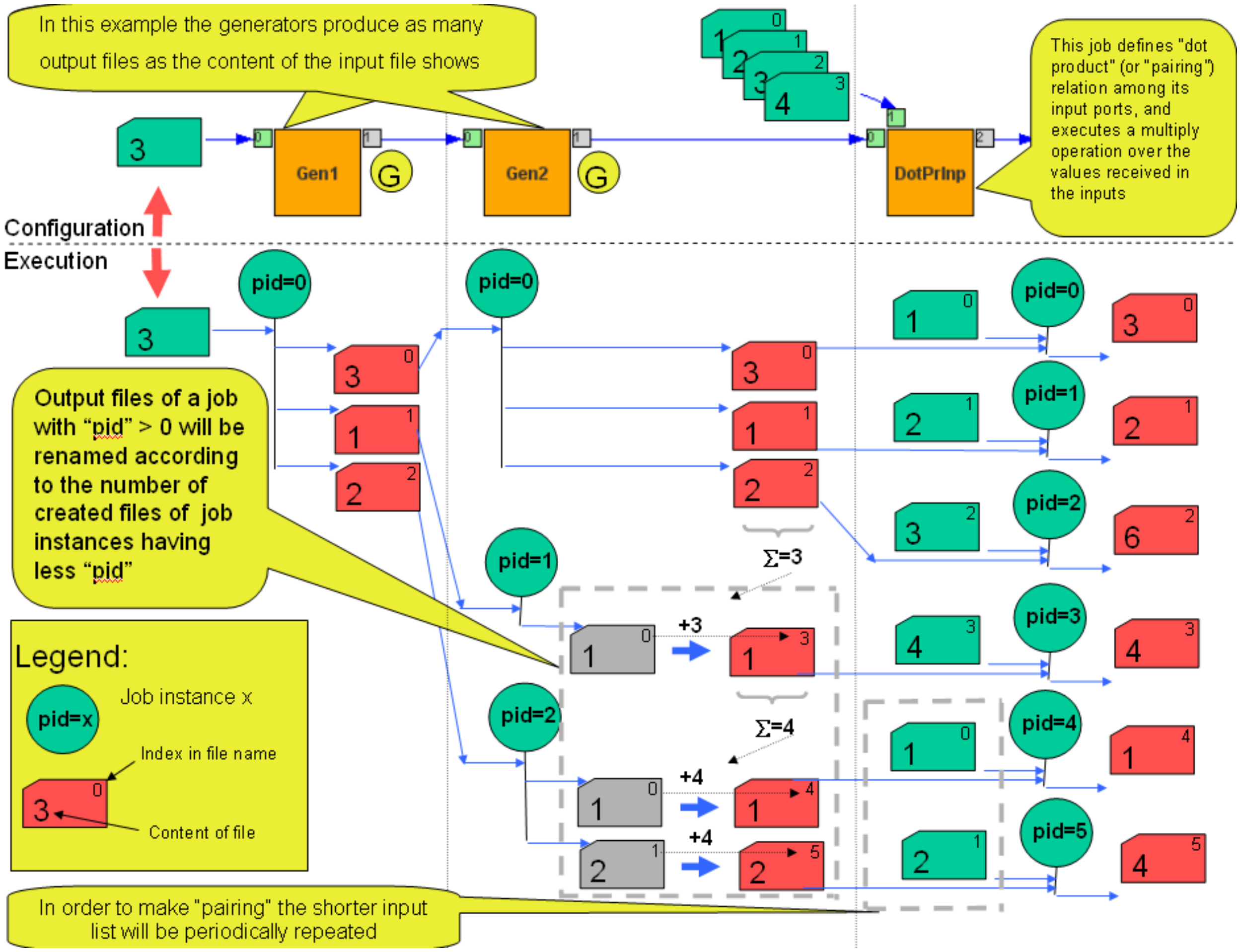
Workflow Interpretation Example (Appendix IV)

The example below shows a three job workflow (see upper part of the picture -> "Configuration") which consists of a cascade of Generator jobs (Gen1, Gen2) and a subsequent job DotPrInp.

The common semantics of the example generators Gen1, Gen2 is defined such a way, that each generator job produces in one job step as many output files as the integer value "N" of its input file is, and the values of these output files are the integers 1,2...N in a random order.

In the example a dot product (pairing) relation is described between the input ports of the Job "DotPrInp" which produces in an output file the multiplication of the values read at the inputs.

It is easy to see that during the execution (lower part of the picture -> "Execution") each instance of Gen2 (pid=0,pid=1,pid=2) must be terminated before the any instances of the DotPrInp (pid=0,pid=1,pid=2,pid=3,pid=4,pid=5) would be started.


In this example the generators produce as many output files as the content of the input file shows
This job defines "dot product" (or "pairing") relation among its input ports, and executes a multiply operation over the values received in the inputs
Gen1
Gen2
DotPrInp
G
Configuration
Execution
pid=0
pid=1
pid=2
pid=3
pid=4
pid=5
Σ=3
Σ=4
+3
+4
+4
Output files of a job with "pid" > 0 will be renamed according to the number of created files of job instances having less "pid"
Legend:
pid=x
Job instance x
Index in file name
Content of file
In order to make "pairing" the shorter input list will be periodically repeated

Appendix VI Figure 1 Workflow Interpretation